The Biopython Structural Bioinformatics FAQ

4 Is there a Bio.PDB reference?

Yes, and I'd appreciate it if you would refer to Bio.PDB in publications if you make use of it. The reference is:

> Hamelryck, T., Manderick, B. (2003) PDB parser and structure class implemented in Python. *Bioinformatics*, **19**, 2308-2310.

The article can be freely downloaded via the Bioinformatics journal website (http://www.binf.ku.dk/users/thamelry/references.html

```
resolution=structure.header['resolution']
keywords=structure.header['keywords']
```

The available keys are `name`, `head`, `deposition_date`, `release_date`, `structure_method`, `resolution`, `structure_reference` (maps to a list of references), `journal_reference`, `author` and `compound`

```
    class GlySelect(Select):
        def accept_residue(self, residue):
            if residue.get_nam=,c='GLY'ct):
```

Figure 1: UML diagram of SMCRA architecture of the `Structure` object. Full lines with diamonds denote aggregation, full lines with arrows denote referencing, full lines

What is a model id?

(see Fig. 1). Each `Atom` object in a `DisorderedAtom` object can be uniquely indexed using its altloc specifier. The `DisorderedAtom` object forwards all uncaught method calls to the selected Atom object, by default the one that represents the atom with with the highest occupancy. The user can of course change the selected `Atom` object, making use of its altloc specifier. Ioa atom39446(Disar)-7er39446its represected

How do I measure torsion angles?

Again, this can easily be done via the vector representation of the atomic coordinates,

```
print sup.rms
# Apply rotation/translation to the moving atoms
sup.apply(moving)
```

How do I superimpose two structures based on their active sites?