The Biopython Structural Bioinformatics FAQ

Bioinformatics center
Institute of Molecular Biology
University of Copenhagen
Universitetsparken 15, Bygning 10
DK-2100 København Ø
Denmark
thamelry@binf.ku.dk
http://www.binf.ku.dk/users/thamelry/

1 Introduction

The Biopython Project is an international association of developers of freely available Python (http://www.python.org) tools for computational m Biolousl20(Biolur5459(Python)]TJ-165.987

Judging from requests for features and information, Bio.PDB is also used by several LPCs (Large Pharmaceutical Companies :-).

4 Is there a Bio.PDB reference?

How do I extract a specific `Atom/Residue/Chain/Model` from a Structure?

Easy. Here are some examples:

```
model=structure[0]
chain=model['A']
residue=chain[100]
atom=residue['CA']
```

Note that you can use a shortcut:

```
atom=structure[0]['A'][100]['CA']
```

What is a model id?

The model id is an integer which denotes the rank of the model in the PDB/mmCIF file. The model is starts at 0. Crystal structures generally have only one model (with id 0), while NMR files usually have several models.

What is a chain id?

The chain id is specified in the PDB/mmCIF file, and is a single character (typically a letter).

What is a residue id?

```
# Calculate classical coordination number exp_fs=hse.calc_fs_exposure(model)
# Print HSEalpha for a residue
print exp_ca[some_residue]
```

How do I map the residues of two related structures onto each other?

First, create an alignment file in FASTA format, then use the `StructureAlignment` class. This class can also be used for alignments with more than two structures.

How do I test if a Residue object is an amino acid?

Use `is_aa(residue)`.

Can I do vector operations on atomic coordinates?

`Atom` objects `return` a `Vector`