

# penm package

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The **penm** package contains functions to build Elastic Network Models (ENM) of proteins and to perturb them. Thus, **penm** stands for Perturbing Elastic Network Models.

## Usage

### Set up the ENM for a protein

First, read a pdb file using `bio3d::read.pdb` to generate a `pdb` object for a protein. Then, create the `prot` object, that contains the full ENM analysis.

```
bio3d::read.pdb("data-raw/2acy_A.pdb") # read a pdb file
prot <- set_enm(pdb, node = "calpha", model = "anm", d_max = 10.5, frustrated = FALSE)
```

In this example, network nodes are placed at  $C_\alpha$  coordinates, the model used is Bahar's Anisotropic Network Model ("anm") with a cut-off distance to define contacts of `d_max = 10.5`. `frustrated` indicates whether to add frustrations to the model.

## Package architecture

### enm dependencies

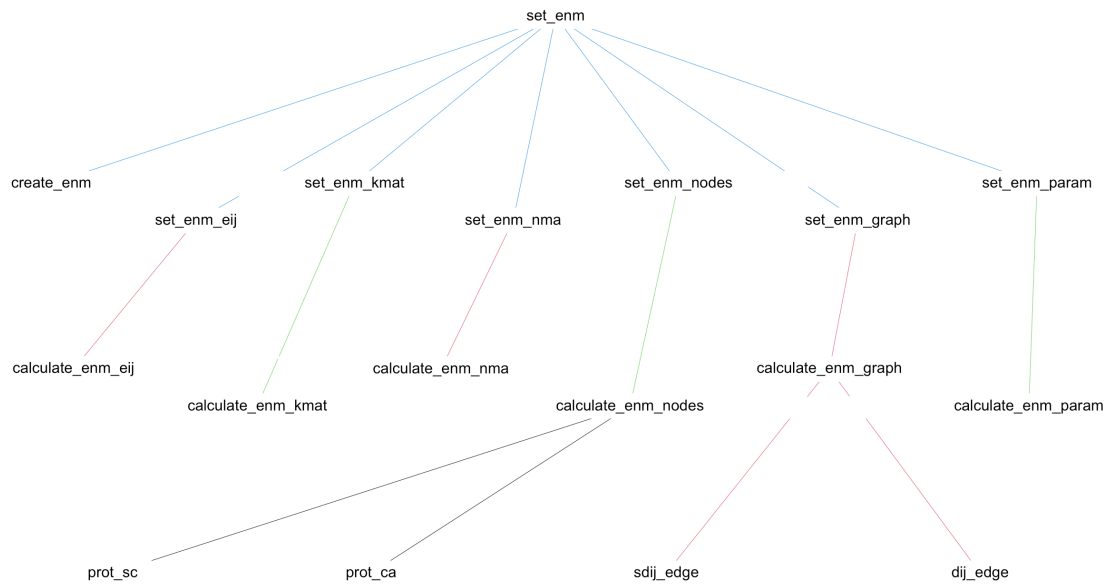


Figure 1: Dependencies of `set_enm()`.

### penm dependencies



Figure 2: Dependencies of `get_mutant_site()`