

# 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_prot(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

- `set_prot(pdb, node, model, d_max, frustrated)`
  - `nodes(pdb, node)`
    - \* `prot_ca(pdb)`
    - \* `prot_sc(pdb)`
      - `residue.coordinates(pdb)`
      - `residue.bfactors(pdb)`
  - `enm_from_xyz(xyz, pdb_site, model, d_max, frustrated)`
    - \* `enm_graph_xyz(xyz, pdb_site, model, d_max)`
      - `my_as_xyz(xyz)`
      - `kij(dij, d_max)`
      - `dij_edge(xyz, i, j)`
      - `sdi_j = sdi_j_edge(pdb_site, i, j)`
    - \* `eij <- eij_edge(xyz, i, j)`
      - `my_as_xyz(xyz)`
    - \* `kmat_graph(graph, eij, nsites, frustrated)`

### penm dependencies

- `get_mutant_site(wt, site_mut, mutation, seed, wt0, mut_sd_min, dl_sigma, update_enm, model, d_max, frustrated)`
  - mutates the graph
  - `get_force(wt, mut)`
  - calculates `dxyz`
  - if (`update_enm`): \* `mutate_enm(mut, model, d_max, frustrated)`
    - \* `mutate_graph(prot, model, d_max)`
      - `enm_graph_xyz(xyz, pdb_site, model, d_max)`
    - \* `mutate_eij(prot)`
      - `eij_edge(xyz, i, j)`
    - \* `kmat_graph(graph, eij, nsites, frustrated)`
    - \* `enm_nma(kmat)` # recalculate normal modes etc. `nma <- enm_nma(prot $\times$ enmkmat)` #returns mode, eval, cmat, umat
  - if (!`update_enm`):
    - \* `dij_edge(xyz, i, j)`