

Function declarations

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enm.R

- `set_enm <- function(pdb, node, model, d_max, frustrated)`
- `create_enm <- function()`
- `set_enm_param <- function(prot, node, model, d_max, frustrated)`
- `set_enm_nodes <- function(prot, pdb)`
- `set_enm_graph <- function(prot)`
- `set_enm_eij <- function(prot)`
- `set_enm_kmat <- function(prot)`
- `set_enm_nma <- function(prot)`
- `calculate_enm_nodes <- function(pdb, node)`
- `prot_sc <- function(pdb)`
- `prot_ca <- function(pdb)`
- `calculate_enm_graph <- function(xyz, pdb_site, model, d_max)`
- `dij_edge <- function(xyz,i,j)`
- `sdij_edge <- function(pdb_site,i,j)`
- `calculate_enm_eij <- function(xyz,i,j)`
- `calculate_enm_kmat <- function(graph, eij, nsites, frustrated)`
- `calculate_enm_nma <- function(kmat, TOL = 1.e-5)`

penm.R

- `get_mutant_site <- function(wt, site_mut, mutation = 0, mut_model = "lfenm", mut_dl_sigma = .3, mut_sd_min = 2, seed = 241956)`
- `get_mutant_site_lfenm <- function(wt, site_mut, mutation, mut_dl_sigma, mut_sd_min, seed)`
- `get_mutant_site_scfenm <- function(wt, site_mut, mutation, mut_dl_sigma, mut_sd_min, seed)`
- `get_delta_lij <- function(wt, site_mut, mut_sd_min, mut_dl_sigma)`
- `get_dxyz <- function(wt, delta_lij)`
- `get_force <- function(wt, delta_lij)`
- `mutate_enm <- function(prot)`
- `mutate_graph <- function(prot)`
- `enm_update <- function(...)`