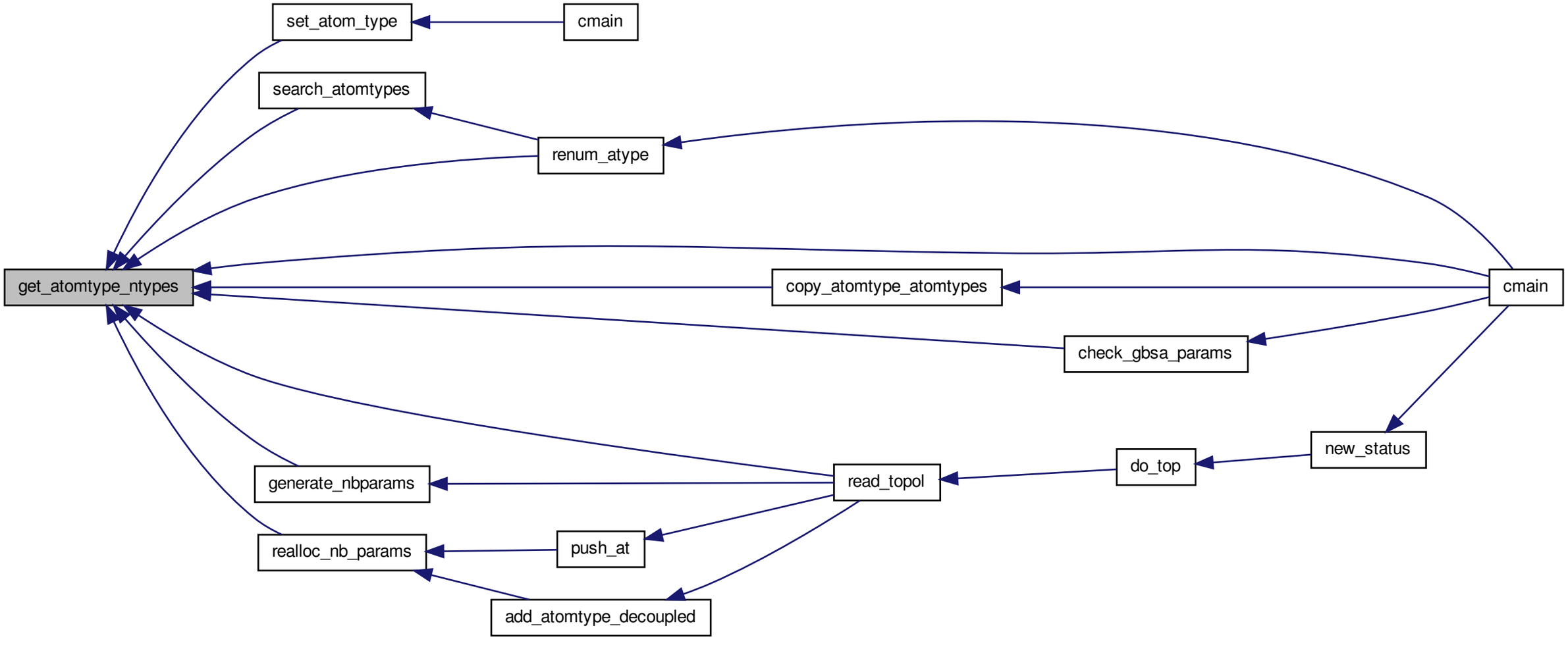
set_atom_type
cmain
search_atomtypes
renum_atype
get_atomtype_ntypes
copy_atomtype_atomtypes
cmain
check_gbsa_params
new_status
do_top
generate_nbparams
read_topol
realloc_nb_params
push_at
add_atomtype_decoupled