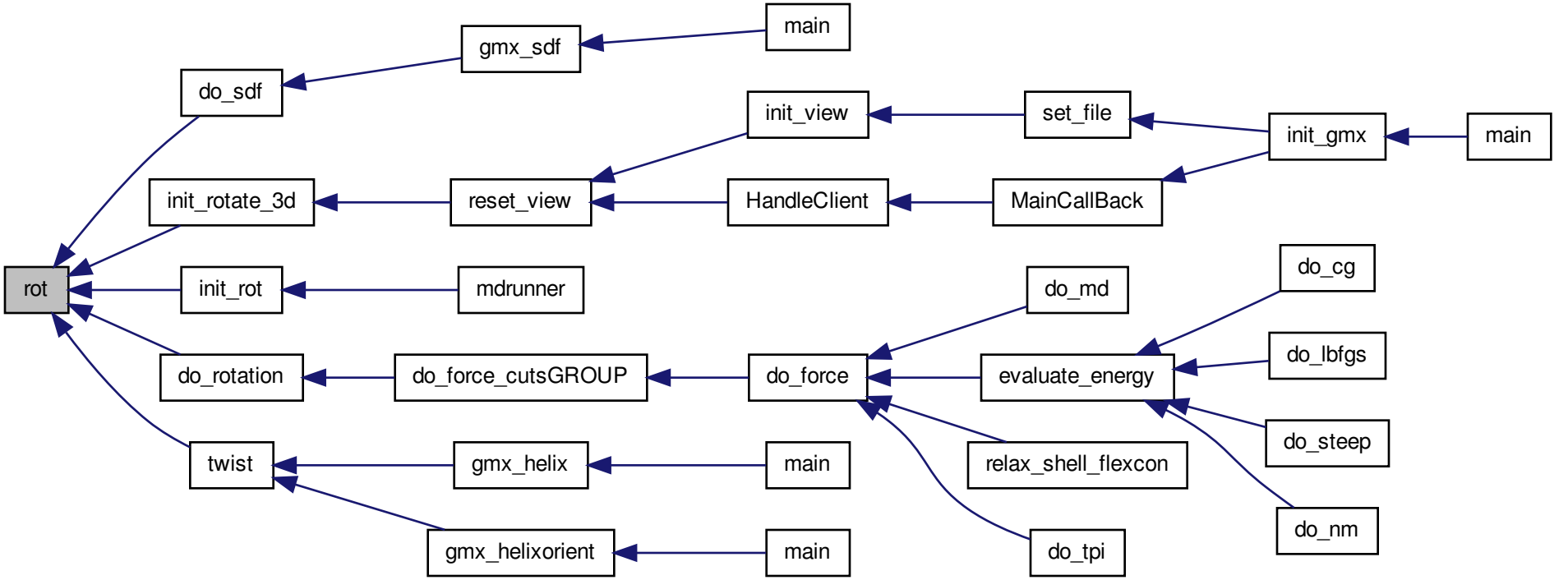
rot
do_sdf
gmx_sdf
main
init_rotate_3d
reset_view
init_view
set_file
init_gmx
main
HandleClient
MainCallBack
init_rot
mdrunner
do_rotation
do_force_cutsGROUP
do_force
do_md
evaluate_energy
do_cg
do_lbfgs
do_steep
do_nm
relax_shell_flexcon
do_tpi
twist
gmx_helix
main
gmx_helixorient
main