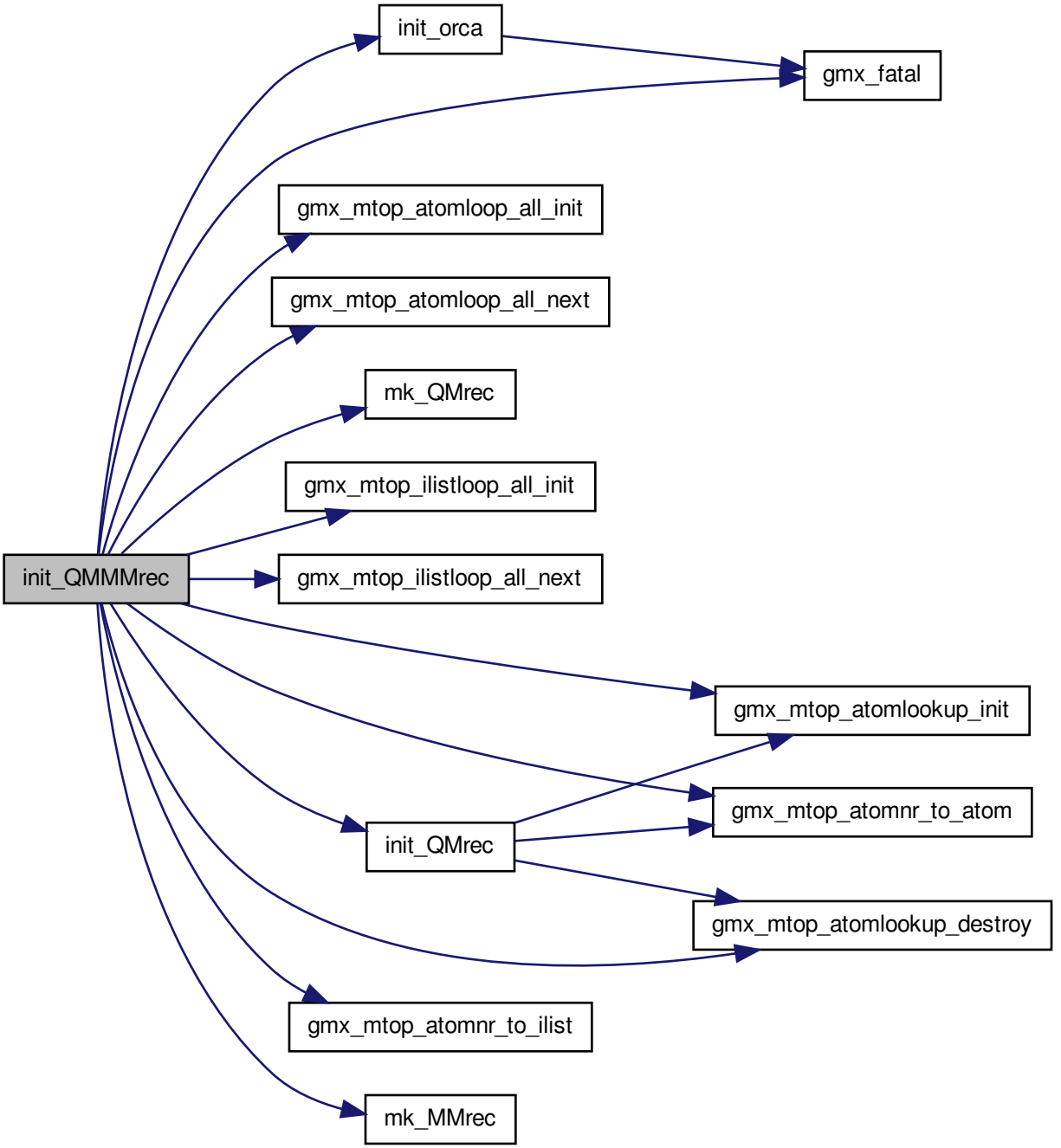
init_orca
gmx_fatal
gmx_mtop_atomloop_all_init
gmx_mtop_atomloop_all_next
mk_QMrec
gmx_mtop_ilistloop_all_init
init_QMMMrec
gmx_mtop_ilistloop_all_next
gmx_mtop_atomlookup_init
gmx_mtop_atomnr_to_atom
init_QMrec
gmx_mtop_atomlookup_destroy
gmx_mtop_atomnr_to_ilist
mk_MMrec