

TRAJ

```
graph TD; TRAJ[TRAJ] --- input[input]; TRAJ --- geom[geom]; TRAJ --- QM[QM]; TRAJ --- restart[restart]; QM --- runQM[runQM.sh]; QM --- MOLPRO[MOLPRO.template]; QM --- SH2PRO[SH2PRO.inp];
```

input

geom

QM

runQM.sh

MOLPRO.template

SH2PRO.inp

restart