

TRAJ

```
graph TD; TRAJ[TRAJ] --- input[input]; TRAJ --- geom[geom]; TRAJ --- QM[QM]; TRAJ --- restart[restart]; QM --- runQM[runQM.sh]; QM --- template[MOLCAS.template]; QM --- resources[MOLCAS.resources];
```

input

geom

QM

runQM.sh

MOLCAS.template

MOLCAS.resources

restart