bash command

```
$ # If using the conda install or have no mpi compiled version:
$ sander -O -i min.in -o min.out -c start.rst7 -p complex.parm7 -inf min.mdinfo -r min.ncrst
$
$ # If compiled with mpi:
$ mpirun -np NUM_CORES sander.MPI -O -i min.in -o min.out -c start.rst7 -p complex.parm7 -inf min.mdinfo -r min.ncrst
$
$ # If using the full version of amber with GPU support:
$ pmemd.cuda -O -i min.in -o min.out -c start.rst7 -p complex.parm7 -inf min.mdinfo -r min.ncrst
$ ### NOTE: Often the pmemd version struggles if large clashes are present. If you get an error, try switching to sander.
```