GROMACS - Task #2735

Allow gmx_genrestr to write correct position restraints for molecules after the first molecule

11/05/2018 07:50 PM - Joe Jordan

Status:	New
Priority:	Normal
Assignee:	Joe Jordan
Category:	preprocessing (pdb2gmx,grompp)
Target version:	future
Difficulty:	simple

Description

If you want to have position restraints for multiple chains in a protein, this is currently not allowed by gmx_genrestr. There is no reason for this and it is a simple change to a single line of gmxana/gmx_genpr.cpp.

With the current code,

```
for (i = 0; i < igrp; i++)
{
    fprintf(out, "%4d %4d %10g %10g %10g\n",
            ind_grp[i]+1, 1, fc[XX], fc[YY], fc[ZZ]);
}
```

the attached script fails to make the B chain restraints. But with a simple change,

```
for (i = 0; i < igrp; i++)
{
    fprintf(out, "%4d %4d %10g %10g %10g\n",
            i+1, 1, fc[XX], fc[YY], fc[ZZ]);
}
```

the script runs successfully. Additionally, the second version is the way writing position restraints (for all heavy atoms) in pdb2gmx works.

I might argue that this is actually a bug, but perhaps there may be some reason it needs to work this way that I don't know about.

History

#1 - 11/05/2018 07:57 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2735.
Uploader: Joe Jordan (e.jjordan12@gmail.com)
Change-Id: gromacs~master~Ifd849020da98b8052f0f965e53a079c6bddfc2d5
Gerrit URL: https://gerrit.gromacs.org/8654

#2 - 11/09/2018 12:19 PM - Joe Jordan

- File posre.sh added

I tested this to make sure that mdrun also works and everything seems fine. I created a slightly more elaborate script to demonstrate this. I think it might be a good idea to turn this script into an integration test using the test fixtures and starting from a suitably equilibrated box.

#3 - 12/11/2019 09:26 AM - Joe Jordan

- Target version changed from 2020 to future

Files

posre.sh	915 Bytes	11/05/2018	Joe Jordan
chainTer.pdb	19.7 KB	11/05/2018	Joe Jordan
ca.mdp	39 Bytes	11/05/2018	Joe Jordan
posre.sh	1.38 KB	11/09/2018	Joe Jordan