

GROMACS - Feature #1900

Implement some new errors in grompp

02/12/2016 02:10 PM - Mark Abraham

Status:	New
Priority:	Normal
Assignee:	
Category:	preprocessing (pdb2gmx,grompp)
Target version:	
Difficulty:	uncategorized
Description	
While discussing https://gerrit.gromacs.org/#/c/5606/6..8/src/gromacs/mdlib/csettle.cpp , we suggested such a check also take place in grompp	
Now that pull groups might get identified with strings like "8 1 1 2 3 4" we should check that the pairings that result are not between identical groups such that they are sure to produce zero-length displacement vectors.	

History

#1 - 02/13/2016 09:42 PM - Berk Hess

Note that these are errors, not warnings.

For settle we should also check that all masses are identical for all water topologies, including B-states.

#2 - 06/01/2016 01:58 PM - Mark Abraham

- Subject changed from *Implement some new warnings in grompp* to *Implement some new errors in grompp*

#3 - 06/01/2016 01:58 PM - Mark Abraham

- Assignee deleted (Mark Abraham)

Looking unlikely to be ready in time for 2016

#4 - 06/22/2016 05:20 PM - Mark Abraham

- Target version deleted (2016)