

GROMACS - Bug #2427

gmx select gives syntax error for selection involving evaluating simple arithmetic expression

02/27/2018 05:15 PM - Viveca Lindahl

Status: New	
Priority: Normal	
Assignee:	
Category: selections	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018	
Description	
gmx_debug select -s topol.tpr -select "n=1+1; resid n" -on selected.ndx	
has output:	
[...]	
Program: gmx select, version 2018.1-dev-20180227-8223d56	
Source file: src/gromacs/commandline/cmdlineparser.cpp (line 276)	
Function: void gmx::CommandLineParser::parse(int*, char**)	
Error in user input:	
Invalid command-line options	
In command-line option -select	
Invalid selection 'resid n'	
Near 'n'	
syntax error	
[...]	
I'm assuming this should not be a syntax error. Replacing "n=1+1" in the selection string by n=2 doesn't give rise to an error.	