

GROMACS - Bug #288

out.gro problem

02/09/2009 04:34 AM - Fan Jiang

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description Hello, I am trying to use genbox program to add water to my piptide: #genbox -cp out -cs -p 1qs4a -o b4em But the result always shows: Fetal erro: A coordinate in file out.gro does not contain a '.' I have pasted my files into attechment. Could you kindly tell me what's wrong in my process? Many thanks, Best wishes, Fan Jiang	

History

#1 - 02/09/2009 07:58 AM - Erik Lindahl

Not a bug, user input error.