

## GROMACS - Bug #97

### pdb2gmx produces unusable ARGN

08/18/2006 03:05 PM - Erik Marklund

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> David van der Spoel	
<b>Category:</b> mdrun	
<b>Target version:</b> 3.3_rc1	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	
<b>Description</b>	
Neutralizing arginines (ARGN) with virtual sites in pdb2gmx generates constraints between CZ and HH1. Such constraints have no parameters, grompp sets them to zero length and gives warnings, and mdrun subsequently crashes.	

### History

#### #1 - 04/14/2007 07:24 PM - David van der Spoel

Hi Erik,

could you please upload an exampl pdb file and command line?

#### #2 - 04/16/2007 11:02 AM - Erik Marklund

Created an attachment (id=144)

Ubiquitin. Makes faulty top-file.

#### #3 - 04/16/2007 11:02 AM - Erik Marklund

I can't remember exactly which files I used or exactly what I did, but I managed to reproduce the error in the following way:

```
pdb2gmx -f 1UBQ.pdb -o tst -i tst -p tst -arg -vsite hydrogens
```

I chose the OPLS-force field and set the arginines to neutral.

From the gro-file tst.gro:

```
...
42ARGN CZ 737 2.713 3.242 2.657
42ARGN NH1 738 2.763 3.366 2.646
42ARGN HH1 739 2.690 3.432 2.660
42ARGN NH2 740 2.581 3.230 2.673
42ARGN HH21 741 2.539 3.139 2.675
42ARGN HH22 742 2.524 3.311 2.683
...
```

From the constraint section of tst.top:

```
...
737 739 2
...
```

Running grompp afterwards yields a bunch of warnings about the constraints:

```
grompp -f vacuumsim/em.mdp -c tst.gro -p tst.top -o grompp_tst -po grompp_tst
```

```
...
WARNING 2 [file "tst.top", line 2706]:
No default Constr. No Conn. types, using zeroes
WARNING 3 [file "tst.top", line 2731]:
No default Constr. No Conn. types, using zeroes
WARNING 4 [file "tst.top", line 2782]:
No default Constr. No Conn. types, using zeroes
WARNING 5 [file "tst.top", line 2789]:
No default Constr. No Conn. types, using zeroes
...
```

(Warning 1 arose from using a slightly unsuited mdp-file for this test case and shouldn't affect the problem with the constraints.)

I didn't try starting the simulation this time, since I'm quite convinced it'll crash.

All of the above was done using gromacs 3.3.2b. I'll upload the pdb-file.

#### #4 - 09/07/2007 01:00 PM - David van der Spoel

This will be fixed automagically when you build the new genvsite algorithms. It could also be resolved by simply adding a distance to the ffoplsaabon.itp similar to the other constraint lengths that are there.

#### Files

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1UBQ.pdb	58.8 KB	04/16/2007	Erik Marklund
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