

GROMACS - Bug #1802

g_chi segfault with system

08/11/2015 11:30 PM - Rafael de la Vega

Status: Closed	
Priority: Normal	
Assignee: Justin Lemkul	
Category: analysis tools	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 4.6.5	
Description	
When I run g_chi on this system, it segfaults, usually after writing the chiXXX.xvg files. I tried removing the non-standard residue, that didnt help.	

Associated revisions

Revision e7dc5714 - 08/14/2015 03:05 AM - Justin Lemkul

Avoid segmentation fault in gmx chi.

If a system containing a custom residue is being analyzed, gmx chi would seg fault if that residue was not in residuetypes.dat. This can occur, for instance, when the topology is created in some directory and analysis in another, or if the analysis is done on a different machine.

Fixes #1802

Change-Id: I85df855381c8e233020fd1e1f73165d4e1215ab9

History

#1 - 08/11/2015 11:56 PM - Mark Abraham

Can you please describe what's in your system?

#2 - 08/12/2015 12:05 AM - Rafael de la Vega

The system is a protein with a cysteine/flavin covalent adduct as a non-standard amino acid, called FMC. The force field is amber99-ildn.

#3 - 08/12/2015 01:07 PM - Mark Abraham

g_chi has a lot of options - which ones are you using?

#4 - 08/12/2015 10:45 PM - Rafael de la Vega

I tried a lot of options, none of them worked. I did get the system to work without the non-standard amino acid, so I think the problem is with the FMC residue somehow.

#5 - 08/12/2015 11:17 PM - Justin Lemkul

Trying a lot of things doesn't help anyone debug the issue. We need an exact command that you're issuing in order to reproduce it.

#6 - 08/12/2015 11:41 PM - Rafael de la Vega

I must have been a little unclear, any combination of options that I tried caused a segfault, including just the defaults. The error is reproducible on multiple linux machines, including a campus cluster

#7 - 08/13/2015 05:57 PM - Justin Lemkul

- Category set to analysis tools

- Status changed from New to Feedback wanted

I suspect you did not add FMC to residuetypes.dat and define it as a Protein residue. The failure comes from gmx_residue_type_get_index(), which sets the residue index in dlist[] in gmx chi. In the case that FMC is not defined as Protein, the index is set to -1 and you get a seg fault. Adding FMC

to residuetypes.dat solves the problem. I don't know if there is a graceful solution to this, really, but in principle we could check for (dlist[i].index == -1) and exit with an error if that is the case.

#8 - 08/14/2015 12:32 AM - Rafael de la Vega

That did the job, thanks. I did have FMC in a copy of residuetypes.dat but the file got lost in the creation of new directories.

#9 - 08/14/2015 02:29 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1802](#).
Uploader: Justin Lemkul (jalemkul@vt.edu)
Change-Id: I85df855381c8e233020fd1e1f73165d4e1215ab9
Gerrit URL: <https://gerrit.gromacs.org/4994>

#10 - 08/14/2015 03:06 AM - Justin Lemkul

- Status changed from Feedback wanted to Fix uploaded
- Assignee set to Justin Lemkul

#11 - 08/15/2015 10:30 PM - Justin Lemkul

- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset [e7dc5714e7d0f791ac2b82f40347dd25bbbb87a7](#).

#12 - 04/03/2016 11:42 PM - Erik Lindahl

- Status changed from Resolved to Closed

Files

test.xtc	7.26 MB	08/11/2015	Rafael de la Vega
topol.tpr	1.22 MB	08/11/2015	Rafael de la Vega