Gromacs - Feature #1161
Fix AMBER GB/SA parameters
02/26/2013 04:00 PM - Justin Lemkul

Status: Closed
Priority: Normal
Assignee: Erik Lindahl
Category: preprocessing (pdb2gmx,grompp)
Target version: 5.0

Description
As noted in [[http://lists.gromacs.org/pipermail/gmx-users/2012-November/076230.html]], agreement between GROMACS GB/SA and AMBER11 is improved with the posted modifications to gbsa.itp.

Associated revisions
Revision 3c094c1 - 06/25/2014 07:27 PM - Erik Lindahl
Updated Amber GBSA parameters

Updated parameters according to Per Larsson's post on gmx-users in November 2012 (076230.html) that found energies to agree to at least within 0.2kJ/mol (OK, not great).

Fixes #1161.

Change-id: i1666238c332fb9d8cc82ab6faea672e016d78757

History
#1 - 02/26/2013 04:08 PM - Justin Lemkul
- Target version changed from 4.6.2 to future

Set to "future" since this is the kind of thing that will affect results and is probably not good for a patch release.

#2 - 03/06/2013 02:41 PM - Berk Hess
- Assignee changed from Berk Hess to Erik Lindahl

#3 - 01/10/2014 08:35 PM - Szilárd Páll
How about doing this in 5.0?

#4 - 06/09/2014 09:07 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1161.
Uploader: Erik Lindahl (erik@kth.se)
Change-id: i1666238c332fb9d8cc82ab6faea672e016d78757
Gerrit URL: https://gerrit.gromacs.org/3562

#5 - 06/09/2014 09:07 PM - Erik Lindahl
- Status changed from New to Fix uploaded
Updated link to mailing list post is below:

https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2012-November/076230.html

Can not find any website that has the amber parameters.

#7 - 06/26/2014 10:14 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#8 - 06/26/2014 10:14 PM - Erik Lindahl
- Status changed from Resolved to Closed

#9 - 07/15/2014 09:16 AM - Teemu Murtola
- Target version changed from future to 5.0