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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Erik Lindahl</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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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 3c09f4c1 - 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

#6 - 06/19/2014 01:26 PM - David van der Spoel
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