Gromacs - Bug #1859

make_ndx does not work
11/24/2015 02:16 PM - David van der Spoel

<table>
<thead>
<tr>
<th>Status</th>
<th>Resolved</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version</td>
<td>5.1.2</td>
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</tbody>
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Affected version - extra info:

| Affected version | git master        |

Description
Using either of the 'a' or 'r' or 't' options do not work anymore in the master version of make_ndx. This could be related to a patch removing the NOTSET construct from legacyheaders/types.

gmx make_ndx -f conf.pdb << EOF
a H
EOF
reproduces the problem.

Associated revisions
Revision de9f5bbe - 11/24/2015 02:49 PM - David van der Spoel
Fixes newly introduced bug in make_ndx.

After cleanup removing "NOTSET" from general include files a bug was introduced in make_ndx not being able to generate groups based on atom name, residue name or atom type.

Fixes #1859
Change-Id: i5ccca69ca31ae9d53f7473bcd9e6864db9a66fc8

History
#1 - 11/24/2015 02:51 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1859
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: i5ccca69ca31ae9d53f7473bcd9e6864db9a66fc8
Gerrit URL: https://gerrit.gromacs.org/5375

#2 - 11/24/2015 10:00 PM - David van der Spoel
- Status changed from New to Resolved

Applied in changeset de9f5bbe8c29d04ae3d5d5f412b408e76781d25a.

Files
conf.pdb 4.25 KB 11/24/2015 David van der Spoel

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