As reported by schlesi@uni-mainz.de for the COOH terminal group one of the angles (the one including two carbons and the oxygen which carries the hydrogen) does not get overwritten by aminoacids.c.tdb.

Ok, somewhat slower:
Used ASPH as a test molecule and chose a -COOH capping group.

From aminoacids.rtp:

```plaintext
[ ASPH ]
[ atoms ]
... C  C  0.450  3
  O  O  -0.450  3
...
[ angles ]
; ai  aj  ak  gromos type
... CA  C  O  ga_30
...
```

From aminoacids.c.tdb:

```plaintext
[ COOH ]
[ replace ]
 C  C  C  12.011  0.33
 O  O  OA  15.9994 -0.288
 OXT OT O  15.9994 -0.45
...
[ angles ]
 O  C  OT  ga_33
 C  O  HO  ga_12
 CA  C  O  ga_19
 CA  C  OT  ga_30
```

This mean that from [ASPH] the atom named O with the type O should exchange by an atom named O with the typ OA. Additionally the angle for CA-C-O should change form ga_30 to ga_19

Result from pdb2gmx:

```
; It was generated using program:
; pdb2gmx - VERSION 4.6.5
;
; Command line was:
; pdb2gmx -f asp.pdb -o asp.gro -p asp.top -asp -ter
...
; Include forcefield parameters
#include "gromos53a5.ff/forcefield.itp"
```
... [atoms]
...
10 C 1 ASPH C 4 0.658 12.011 ;
11 O 1 ASPH OT 4 -0.45 15.9994 ;
12 OA 1 ASPH O 4 -0.611 15.9994 ;
...
[angles]
...
4 10 11 2 ga_30
4 10 12 2 ga_30 ...

First line from the posted [angle] is the right angle with the atom named OT.
In the second line we have still the angle from [ASPH] which doesn't get replaced by the angle from [COOH].

I tested this with GMX 4.6.5 and GMX 4.0.7 -> Think every version from GMX 4.X.Y series is affected.
Also tested it with the gromos53a5, gromos53a6, gromos43a1 force fields -> Think every gromos force field might be affected.

for GMX 4.0.7 and GMX 4.6.5 is a typo in the aminoacids.rtp file (but i would assume that it affects the whole 4.X.Y series).

[ ASPH ]
[atoms]
...
OD1 opls_269 -0.530 3
OD2 opls_268 -0.440 4
HD2 opls_270 0.450 4
...

The charges of OD1 and OD2 should be exchanged (from ffnonbonded.itp):

opls_268 OH 8 15.99940 -0.530 ...
opls_269 O_3 8 15.99940 -0.440 ...

For GLUH and the COOH terminal group everything is fine.

Associated revisions

Revision 592f8422 - 06/20/2014 04:25 PM - Rossen Apostolov
Fixed typo in oplsaa ASPH charges.
Part of #1395.
Change-Id: i03c88c8377affadc629c7b9a04d5e8ddd1cb946a

Revision 8ebd438f - 06/24/2014 02:24 PM - Erik Lindahl
Make sure duplicates bondeds are set from hackblocks

Previously the rtp file could end up containing two entries when the N/C termini databases added interactions.
These were then quicksorted, which could make the assignment random. We now check for duplicates and discard the rtp entry in favor of the hackblock.
Fixes #1395.
Change-Id: i505cfbb7e6c8e8050e6e2935cc417e49a515d8d8

11/25/2015
History

#1 - 06/19/2014 03:15 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1395.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I03c88c8377affadc629c7b9a04d5e8dd1cb946a
Gerrit URL: https://gerrit.gromacs.org/3630

#2 - 06/19/2014 03:16 PM - Rossen Apostolov
The patch above fixes only the opls typo. I don't know what's cause of the first part of the report.

#3 - 06/23/2014 02:05 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1395.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I505cfbb7e6c8e8050e6e2935cc417e49a515d8d8
Gerrit URL: https://gerrit.gromacs.org/3656

#4 - 06/23/2014 02:07 AM - Erik Lindahl
- Status changed from New to Fix uploaded

#5 - 06/24/2014 02:11 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1395.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I8045d4ae8cde681607b21ceedf0810
Gerrit URL: https://gerrit.gromacs.org/3678

#6 - 06/24/2014 08:29 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#7 - 06/24/2014 08:29 PM - Erik Lindahl
- Status changed from Resolved to Closed