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:

[ 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:

[ 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: i03c88c8377affadc629c7b9a04d5e8dd1cb946a

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: i505cfbb7e6c8e050e6e2935cc417e49a515d8d8

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: i8045d4ae8cde68160fd3590476a7b21ec2f0810
Gerrit URL: https://gerrit.gromacs.org/3679

#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