GROMACS - Bug #2511

Editconf mead generated pqr file didn't follow pqr spec

05/22/2018 04:09 PM - zhiyi wu

Status:	Closed		
Priority:	High		
Assignee:			
Category:			
Target version:	2018.2		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018		

Description

When using editconf to generate pqr files.
gmx editconf -f enmin.tpr -mead system.pqr
The generated pqr file didn't follow the pqr file format specification (https://apbs-pdb2pqr.readthedocs.io/en/latest/formats/pqr.html), where:

1. The pqr shouldn't contain atom type at the end of the line
2. There should always be a space separating the columns.

Here is a sample of pqr file.

```
REMARK    The B-factors in this file hold atomic radii
REMARK    The occupancy in this file hold atomic charges
TITLE     system
REMARK    THIS IS A SIMULATION BOX
CRYST1   35.060   34.040   38.990  90.00  90.00  90.00 P 1          1
MODEL        1
ATOM      1  N   MET A   1      81.952  52.151  32.219  0.16  1.62          N
ATOM   7335  N   MET B   1      30.317  32.933  28.543  0.16  1.62          N
ATOM   7855  N   POPEE 474       9.856  33.258  32.940 -0.29  1.65          N
ATOM  10605  N   POPEa 496      37.380  63.975  30.931 -0.29  1.65          N
ATOM  13855  N   POPE0 522      90.878  72.350  68.454 -0.29  1.65          N
ATOM  15105  N   POPE  532      16.405   8.140  68.984 -0.29  1.65          N
TER
ENDMDL
```

As is shown in the snapshot provided, if the residue name has a length of 4 characters (POPE), there will be no space between residue name and chain id (POPE a) instead of (POPEa).

Associated revisions

Revision b0f4bf1d - 06/06/2018 10:24 AM - Paul Bauer

Fix PQR file output

PQR files from editconf were always written as fixed format PDB files
with just the field information added. As pointed out in the linked
redmine, this can violate the PQR file standard if the field lengths are
too long, even though the file would still be a valid PDB.

This adds a slightly different form of the writeout that has a flexible,
PQR conform format.

Fixes #2511

Change-Id: I626380b642a0214970753da289e9c969ce411ea7

History

#1 - 05/22/2018 05:09 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2511.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I626380b642a0214970753da289e9c969ce411ea7
Gerrit URL: https://gerrit.gromacs.org/7929

#2 - 05/22/2018 05:11 PM - Mark Abraham

Can you please share the .tpr file, so we can perhaps agree on how the output should look if/when we fix editconf?

#3 - 05/22/2018 05:15 PM - Mark Abraham

- Status changed from New to Fix uploaded

#4 - 05/22/2018 05:23 PM - zhiyi wu

- File enmin.tpr added

Mark Abraham wrote:

> Can you please share the .tpr file, so we can perhaps agree on how the output should look if/when we fix editconf?

Here is a sample tpr file contain two POPE molecules.
If "gmx editconf -f enmin.tpr -mead system.pqr" was run, the output pqr file will be

```
REMARK    The B-factors in this file hold atomic radii
REMARK    The occupancy in this file hold atomic charges
TITLE     GkApcT YneM POPE POPG in water
REMARK    THIS IS A SIMULATION BOX
CRYST1  109.329   90.329   91.654  90.00  90.00  90.00 P 1           1
MODEL        1
ATOM      1  N   POPEA   1      14.430  46.000  29.240 -0.29  1.65           N
...
ATOM    250 H16Z POPEB   2     100.140   5.340  54.660  0.02  1.10           H
TER
ENDMDL
```

The suggested output which adheres to the pqr spec will be:

```
REMARK    The B-factors in this file hold atomic radii
REMARK    The occupancy in this file hold atomic charges
TITLE     GkApcT YneM POPE POPG in water
REMARK    THIS IS A SIMULATION BOX
CRYST1  109.329   90.329   91.654  90.00  90.00  90.00 P 1           1
MODEL        1
ATOM      1  N   POPE A   1      14.430  46.000  29.240 -0.29  1.65
...
ATOM    250 H16Z POPE B   2     100.140   5.340  54.660  0.02  1.10
TER
ENDMDL
```

#5 - 06/06/2018 10:30 AM - Paul Bauer

- Status changed from Fix uploaded to Resolved

Applied in changeset b0f4bf1d0a83e6bf095d3e557d3a160fe9fac8fc.

#6 - 06/07/2018 01:48 AM - Mark Abraham

- Status changed from Resolved to Closed

- Target version set to 2018.2

Files

enmin.tpr	46.1 KB	05/22/2018	zhiyi wu