

## Issues

| #    | Project                | Tracker | Status             | Priority | Subject  | Assignee            | Updated             | Target version |
|------|------------------------|---------|--------------------|----------|--|---------------------|---------------------|----------------|
| 3404 | GROMACS                | Bug     | Closed             | High     | 2019.6 regression test tarball is missing                                    | Paul Bauer          | 02/28/2020 05:29 PM |                |
| 982  | GROMACS                | Bug     | Closed             | High     | segfault in genion   | Roland Schulz       | 07/31/2012 02:59 AM | 4.6            |
| 970  | GROMACS                | Bug     | Closed             | High     | segfault in tip4pflex test case  | Berk Hess           | 07/26/2012 01:31 AM | 4.6            |
| 3408 | GROMACS                | Bug     | Fix uploaded       | Normal   | Gmxapi* tests segfault in rpmbuild   | Eric Irrgang        | 03/23/2020 01:27 PM | 2020.2         |
| 3294 | GROMACS                | Bug     | New                | Normal   | multiple tests fail on fedora 31   | Paul Bauer          | 02/28/2020 03:12 PM | 2020.2         |
| 3291 | GROMACS                | Bug     | Closed             | Normal   | gmx-2020 tarball misses gmx-completion.bash                                  | Paul Bauer          | 02/11/2020 11:15 AM | 2020.1         |
| 3116 | GROMACS                | Bug     | New                | Normal   | regressiontests/freenenergy core dumps on ppc64le                            | Paul Bauer          | 10/04/2019 10:52 PM |                |
| 2854 | GROMACS                | Bug     | New                | Normal   | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1                        | Paul Bauer          | 02/04/2019 11:17 AM |                |
| 2853 | GROMACS                | Bug     | New                | Normal   | EwaldUnitTests segfault on armv7hl with gcc-9.0.1                            | Paul Bauer          | 02/04/2019 05:34 PM |                |
| 2821 | GROMACS                | Bug     | Closed             | Normal   | Compile with OpenCL fails on i686 and armv7hl                                | Paul Bauer          | 02/08/2019 03:14 PM | 2019.1         |
| 2813 | GROMACS                | Bug     | Closed             | Normal   | regressiontests/complex fails on Fedora30 with x86_64, i686 and other archs. | Berk Hess           | 03/14/2019 02:23 PM | 2019.1         |
| 2734 | GROMACS                | Bug     | In Progress        | Normal   | regressiontests/kernel core dumps on ppc64le                                 | Paul Bauer          | 06/15/2019 04:12 PM | future         |
| 2733 | GROMACS                | Bug     | Blocked, need info | Normal   | MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5      | Paul Bauer          | 01/17/2020 08:40 AM |                |
| 2709 | GROMACS                | Bug     | Closed             | Normal   | pygments cannot be detected with PythonInterp is python3                     | Paul Bauer          | 06/12/2019 05:35 PM | 2019-beta2     |
| 2708 | GROMACS                | Bug     | Closed             | Normal   | gromacs-2019 fails to build with openmpi-2.0.2                               | Mark Abraham        | 10/24/2018 11:44 AM | 2019-beta2     |
| 2589 | GROMACS                | Bug     | Rejected           | Normal   | regressiontests/kernel core dumps on ppc64 (f29)                             |                     | 01/03/2019 11:05 AM |                |
| 2584 | GROMACS                | Bug     | Rejected           | Normal   | regressiontests/complex fails on i686  | Szilárd Páll        | 10/21/2019 06:55 PM | 2019.2         |
| 2533 | GROMACS                | Bug     | Closed             | Normal   | GROMACS fails to build with lmfit-7.0  | Mark Abraham        | 06/13/2018 09:18 AM | 2019           |
| 2484 | TNG trajectory library | Bug     | Closed             | Normal   | Push release tags to github  | Magnus Lundborg     | 01/03/2019 10:57 AM | version 1      |
| 2421 | GROMACS                | Bug     | Closed             | Normal   | EwaldUnitTests and SimdUnitTests fail on ppc64le with gcc-8.0.1              | Mark Abraham        | 01/03/2019 10:57 AM | future         |
| 2403 | GROMACS                | Bug     | Closed             | Normal   | Multidir sim with #mpiranks = 2*#sim fails                                   | Mark Abraham        | 03/01/2018 09:33 AM | 2018.1         |
| 2389 | GROMACS                | Bug     | Rejected           | Normal   | Test don't build with external tinyxml2 version 6                            | Mark Abraham        | 01/03/2019 11:11 AM |                |
| 2366 | GROMACS                | Bug     | Closed             | Normal   | HardwareTopologyTest.NumaCacheSelfconsistency fails on aarch64               |                     | 02/24/2020 03:37 PM | 2020.1         |
| 2365 | GROMACS                | Bug     | Closed             | Normal   | UtilityUnitTests is broken on ppc64le, aarch64, ppc64, s390x and armv7hl     |                     | 12/29/2017 08:42 AM |                |
| 2363 | GROMACS                | Bug     | Closed             | Normal   | CorrelationsTest fails with lmfit-6.2  | David van der Spoel | 12/29/2017 11:41 AM | 2018-rc1       |
| 2251 | TNG trajectory library | Bug     | Closed             | Normal   | git release tag for 1.8.0 missing on github                                  | Magnus Lundborg     | 01/03/2019 11:01 AM |                |
| 2250 | TNG trajectory library | Bug     | Closed             | Normal   | tng_io-configVersion.cmake: has no version                                   | Magnus Lundborg     | 01/03/2019 10:58 AM |                |
| 2073 | GROMACS                | Bug     | Closed             | Normal   | cmake fails with CMAKE_CXX_FLAGS="-Wall -Werror"                             | Mark Abraham        | 01/20/2017 11:33 AM | 2016.2         |

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|------|---------|---------|--------|----------|---|--------------------|---------------------|----------------|
| 1468 | GROMACS | Bug     | Closed | Normal   | boost/assert.hpp:102:47: error: 'noinline' was not declared in this scope | Teemu Murtola      | 07/15/2014 10:37 AM | 5.0            |
| 1452 | GROMACS | Bug     | Closed | Normal   | trxio.h cannot be linked by external packages anymore                     | Roland Schulz      | 04/18/2014 05:38 AM | 5.0            |
| 1370 | GROMACS | Feature | Closed | Normal   | regressiontests/freeenergy fail (timeout) on arm                          | Michael Shirts     | 06/19/2014 03:17 PM | 5.0            |
| 983  | GROMACS | Bug     | Closed | Normal   | segfault in grompp (set_pull_init)  | Michael Shirts     | 07/31/2012 05:20 AM |                |
| 978  | GROMACS | Bug     | Closed | Normal   | Bus error on Mac Os when running g_x2top -quiet -man nroff                | Sander Pronk       | 07/25/2012 01:39 AM | 4.6            |
| 771  | GROMACS | Bug     | Closed | Normal   | cmake overwrites BLAS_LIBRARIES and LAPACK_LIBRARIES                      | Rossen Apostolov   | 09/12/2011 02:03 PM | 4.5.5          |
| 732  | GROMACS | Bug     | Closed | Normal   | executable stacks in sse kernels  | Erik Lindahl       | 06/08/2011 03:49 PM |                |
| 698  | GROMACS | Bug     | Closed | Normal   | cleaning up GMXRC.*   |                    | 10/17/2012 11:08 PM |                |
| 693  | GROMACS | Bug     | Closed | Normal   | who is responsible to merge?  |                    | 04/11/2012 12:10 PM |                |
| 685  | GROMACS | Feature | Closed | Normal   | Wrapper binary  | Teemu Murtola      | 02/24/2014 11:00 AM | 5.0            |
| 588  | GROMACS | Bug     | Closed | Normal   | CMake does not build Fortran and Power6 kernels                           | Erik Lindahl       | 10/08/2010 10:35 AM | 4.5.1          |
| 586  | GROMACS | Bug     | Closed | Normal   | openmm: lib issue   | Erik Lindahl       | 10/05/2010 06:08 PM | 4.5.1          |
| 584  | GROMACS | Bug     | Closed | Normal   | configure: broken check for dlopen  | Christoph Junghans | 10/04/2010 11:10 PM | 4.5.1          |
| 575  | GROMACS | Bug     | Closed | Normal   | error.h was not found on AIX 6.1.3.0                                      | Roland Schulz      | 09/28/2010 06:25 PM | CVS            |
| 563  | GROMACS | Bug     | Closed | Normal   | xlc/gcc warnings  | Erik Lindahl       | 10/08/2010 09:51 AM | CVS            |
| 562  | GROMACS | Bug     | Closed | Normal   | building shared or static libs by default                                 | Christoph Junghans | 11/24/2010 09:45 AM | CVS            |
| 561  | GROMACS | Bug     | Closed | Normal   | power6 kernels are broken   | Christoph Junghans | 09/15/2010 11:57 AM | CVS            |
| 535  | GROMACS | Bug     | Closed | Normal   | g_pme_error: Invalid tMPI_Comm  | Sander Pronk       | 08/31/2010 09:23 PM | CVS            |
| 529  | GROMACS | Bug     | Closed | Normal   | md5.c does not compile under AIX 6.1                                      | Roland Schulz      | 08/30/2010 01:36 PM | CVS            |
| 519  | GROMACS | Bug     | Closed | Normal   | g_energy displays wrong average   | Erik Lindahl       | 08/26/2010 05:01 PM | 4.0            |
| 477  | GROMACS | Bug     | Closed | Normal   | threads do not compile using xlc on aix                                   | Sander Pronk       | 07/22/2010 02:38 PM | CVS            |
| 476  | GROMACS | Bug     | Closed | Normal   | git version check in configure / genversion.sh is broken for non-GNU test | Teemu Murtola      | 08/23/2010 10:01 AM | CVS            |
| 475  | GROMACS | Bug     | Closed | Normal   | power6 kernels do not build   | Erik Lindahl       | 07/27/2010 11:46 AM | CVS            |
| 474  | GROMACS | Bug     | Closed | Normal   | threads linking   | Sander Pronk       | 07/22/2010 01:53 PM | CVS            |
| 473  | GROMACS | Bug     | Closed | Normal   | xml overlinking   | Erik Lindahl       | 07/22/2010 01:54 PM | CVS            |
| 472  | GROMACS | Bug     | Closed | Normal   | gsl overlinking   | Erik Lindahl       | 07/22/2010 01:54 PM | CVS            |
| 471  | GROMACS | Bug     | Closed | Normal   | fftw overlinking  | Erik Lindahl       | 07/22/2010 01:54 PM | CVS            |
| 470  | GROMACS | Bug     | Closed | Normal   | X11 overlinking   | Erik Lindahl       | 07/20/2010 12:08 PM | CVS            |
| 469  | GROMACS | Bug     | Closed | Normal   | libgmxpreprocess missed SHARED_VERSION_INFO                               | Erik Lindahl       | 07/20/2010 12:29 PM | CVS            |
| 453  | GROMACS | Bug     | Closed | Normal   | remove install-exec-hook in src/tools/Makefile.am                         | Teemu Murtola      | 07/25/2010 12:06 PM | CVS            |
| 449  | GROMACS | Bug     | Closed | Normal   | Merge in debian patches   | Christoph Junghans | 08/03/2010 03:45 PM | CVS            |

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| 439  | GROMACS | Bug     | Closed             | Normal   | broken gmx headers   | Christoph Junghans  | 08/22/2010 07:12 PM | CVS            |
| 403  | GROMACS | Bug     | Closed             | Normal   | increase SHARED_VERSION_INFO                                       | Erik Lindahl        | 06/23/2010 04:47 PM | CVS            |
| 401  | GROMACS | Bug     | Closed             | Normal   | check for broken libxml  | Erik Lindahl        | 06/02/2010 04:06 PM | CVS            |
| 395  | GROMACS | Bug     | Closed             | Normal   | Missing lib dependencies for libgmxpreprocess                      | Erik Lindahl        | 02/18/2010 12:57 PM | CVS            |
| 393  | GROMACS | Bug     | Closed             | Normal   | Show git sha1sum as version string                                 | Erik Lindahl        | 02/22/2010 06:16 PM | CVS            |
| 392  | GROMACS | Bug     | Closed             | Normal   | make mdrun/install-mdrun is broken                                 | Erik Lindahl        | 02/18/2010 12:57 PM | CVS            |
| 372  | GROMACS | Bug     | Closed             | Normal   | install htmldoc in htmldir   | David van der Spoel | 02/05/2010 04:42 PM | 4.0            |
| 370  | GROMACS | Bug     | Closed             | Normal   | install pkg-config file for better linking                         | Teemu Murtola       | 07/30/2010 09:05 AM | 4.0            |
| 361  | GROMACS | Bug     | Closed             | Normal   | path buffer overflow in gromacs stable                             | Erik Lindahl        | 11/04/2009 03:26 PM | 4.0            |
| 323  | GROMACS | Bug     | Closed             | Normal   | Compile problem with cyclecounter on sparc 32                      | Erik Lindahl        | 05/10/2009 11:47 AM | CVS            |
| 3380 | GROMACS | Bug     | Resolved           | Low      | IBM VSX checks fail with gcc-10                                    | Erik Lindahl        | 04/30/2020 01:30 PM | 2020.2         |
| 3265 | GROMACS | Bug     | Blocked, need info | Low      | regressiontests/complex fails on ppc64le                           | Erik Lindahl        | 01/09/2020 05:00 PM |                |
| 1886 | GROMACS | Bug     | Rejected           | Low      | master(72a776a27f10c7d0f19cbbae10dd2da78df7c959) fails clang-3.4.0 | Mark Abraham        | 01/19/2016 10:26 PM | 2016           |
| 1152 | GROMACS | Bug     | Rejected           | Low      | parse_n_real out of bounds   | Michael Shirts      | 04/30/2013 05:02 PM |                |