

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-----------------|---------|--------------------|----------|--|----------------|---------------------|----------------------------|
| 1106 | Benchmark suite | Feature | New | Normal | publish benchmark numbers | | 06/19/2014 12:08 PM | |
| 1105 | Benchmark suite | Feature | New | Normal | produce a benchmark suite | | 09/13/2016 10:31 PM | |
| 3448 | GROMACS | Bug | New | Normal | GMX 2020.1 - Multidir simulations can stop at different times when killed by job manager | | 03/23/2020 02:50 PM | |
| 3444 | GROMACS | Bug | Resolved | Normal | do_dssp does not work(gmx 2020 and 2020.1) | Christian Blau | 06/10/2020 02:45 PM | 2020.2 |
| 3443 | GROMACS | Bug | New | Normal | Bonded GPU kernel performance regression with 2020 | | 03/15/2020 08:15 PM | |
| 3442 | GROMACS | Bug | Accepted | Normal | continuing mdrun with -deffnm and pulling does not work | | 03/15/2020 08:33 AM | |
| 3441 | GROMACS | Bug | Resolved | Normal | Ewald surface-epsilon is incorrect | Berk Hess | 03/18/2020 11:15 PM | 2020.2 |
| 3440 | GROMACS | Bug | New | Normal | Multi-nodes run exits with error with openmpi/4.0.0 | | 03/23/2020 02:10 PM | |
| 3413 | GROMACS | Bug | Feedback wanted | Normal | COMM Removal Failure in GROMACS 2020.1 | | 03/12/2020 02:31 PM | |
| 3412 | GROMACS | Bug | New | Normal | Domain decomposition problems with Gromacs >2018 | | 03/06/2020 04:10 PM | |
| 3411 | GROMACS | Bug | New | Normal | Nightly master release build failure | | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3408 | GROMACS | Bug | Fix uploaded | Normal | Gmxapi* tests segfault in rpmbuild | Eric Irrgang | 03/23/2020 01:27 PM | 2020.2 |
| 3405 | GROMACS | Bug | Accepted | Normal | intermittent OpenCL regressiontest failures | | 03/02/2020 11:01 AM | |
| 3403 | GROMACS | Bug | Resolved | Normal | solvation free energy with couple-intramol set to no | | 04/17/2020 04:00 PM | |
| 3398 | GROMACS | Bug | New | Normal | Intermittent failure of non-bonded kernels when run using nvprof | | 02/25/2020 12:14 PM | |
| 3387 | GROMACS | Bug | New | Normal | Death test bug | | 02/20/2020 05:39 PM | |
| 3385 | GROMACS | Bug | New | Normal | FindLibStdCpp.cmake - wrong sanity check for clang | | 03/04/2020 06:59 PM | |
| 3380 | GROMACS | Bug | Resolved | Low | IBM VSX checks fail with gcc-10 | Erik Lindahl | 04/30/2020 01:30 PM | 2020.2 |
| 3368 | GROMACS | Bug | New | Normal | Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue | Vedat Durmaz | 02/05/2020 04:51 PM | future |
| 3334 | GROMACS | Bug | New | Normal | Check for DD when increasing rlist is broken | Berk Hess | 02/25/2020 03:28 PM | 2020.2 |
| 3333 | GROMACS | Bug | New | Normal | Assertion failure when trying to get unit test help | Paul Bauer | 02/25/2020 10:16 AM | 2021-infrastructure-stable |
| 3310 | GROMACS | Bug | Blocked, need info | Low | Thread affinity on Mac OS | | 02/27/2020 11:10 PM | |
| 3309 | GROMACS | Bug | New | Normal | -reprod: checkpoint reading bug and general considerations | | 02/27/2020 10:45 PM | |
| 3305 | GROMACS | Bug | New | Normal | Case gives FPE with Debug build when GPU update is enabled | | 01/21/2020 05:44 PM | |
| 3304 | GROMACS | Bug | New | Normal | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5 | Michael Shirts | 03/01/2020 03:23 PM | 2020.2 |
| 3301 | GROMACS | Bug | New | Normal | pdb2gmx adding hydrogen | | 01/15/2020 10:17 PM | |
| 3294 | GROMACS | Bug | New | Normal | multiple tests fail on fedora 31 | Paul Bauer | 02/28/2020 03:12 PM | 2020.2 |

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| 3284 | GROMACS | Bug | New | Normal | gmx msd cannot output two xvg files as suggested by command line option | Christian Blau | 01/08/2020 04:50 PM | 2021-infrastructure-stable |
| 3281 | GROMACS | Bug | New | Normal | Test data directory GMX_RELEASE_ASSERT triggers | | 01/06/2020 08:07 PM | |
| 3274 | GROMACS | Bug | New | Normal | Remove ARM NEON SIMD | | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug | New | Normal | gmxapi setup.py complains too much | | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3266 | GROMACS | Bug | New | High | gmx density show wrong symmetrize density profile using -symm? | Super duper | 02/28/2020 08:24 AM | 2020.2 |
| 3265 | GROMACS | Bug | Blocked, need info | Low | regressiontests/complex fails on ppc64le | Erik Lindahl | 01/09/2020 05:00 PM | |
| 3249 | GROMACS | Bug | In Progress | Low | cmake bad tests for avx512 on AMD | Erik Lindahl | 02/26/2020 05:00 PM | |
| 3246 | GROMACS | Bug | Accepted | Normal | GPU code misses settle error check, simulation crashes with segfault without any further output | Artem Zhmurov | 12/20/2019 09:52 AM | 2021-infrastructure-stable |
| 3244 | GROMACS | Bug | In Progress | Normal | center of mass motion removal with position restraints can lead to artifacts | Berk Hess | 12/27/2019 10:40 AM | 2021 |
| 3243 | GROMACS | Bug | Feedback wanted | Normal | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning | | 12/27/2019 10:31 AM | |
| 3240 | GROMACS | Bug | New | Normal | segv with GPU DD direct communication with GPU update and -dlb off | | 01/15/2020 06:16 PM | |
| 3239 | GROMACS | Bug | New | Normal | GPU DD direct communication with GPU update error with RF | | 12/14/2019 05:15 PM | |
| 3234 | GROMACS | Bug | Accepted | Normal | Signal: Floating point exception Signal code: Floating point divide-by-zero | Erik Lindahl | 12/16/2019 03:40 PM | |
| 3233 | GROMACS | Bug | New | Normal | clang-format incorrectly aligning altered function arguments | | 12/13/2019 12:41 PM | |
| 3228 | GROMACS | Bug | New | Normal | gmxapi.commandline_operation should gracefully handle input/output file arguments | Eric Irrgang | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3227 | GROMACS | Bug | New | Normal | solvate does not check return status of gmx_file_rename | | 12/04/2019 01:43 PM | |
| 3223 | GROMACS | Bug | New | Normal | unit test failures give verify -1 | | 12/02/2019 11:58 AM | |
| 3219 | GROMACS | Bug | Resolved | Normal | MANPATH setting is fragile | | 11/02/2020 11:45 AM | |
| 3214 | GROMACS | Bug | New | Normal | Out-of-bounds, overflow and incorrect outputs in gmx spatial | | 11/25/2019 04:11 PM | |
| 3213 | GROMACS | Bug | New | Normal | Having a local residuetypes.dat for custom force field | | 11/21/2019 09:18 PM | |
| 3210 | GROMACS | Bug | New | High | rerun does not reproduce dVcoul/dl | | 12/27/2019 10:45 AM | |
| 3209 | GROMACS | Bug | New | Normal | Interactive molecular dynamics with VMD becomes stuttering after reconnecting | | 11/19/2019 11:36 AM | |
| 3202 | GROMACS | Bug | New | Low | gmx solvate fails to overwrite topology file | | 11/13/2019 02:44 PM | |
| 3198 | GROMACS | Bug | New | Normal | Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0 | | 11/06/2019 12:20 PM | |
| 3197 | GROMACS | Bug | New | Normal | Rework usage of gitattributes and filter in source code formatting scripts | | 11/04/2019 12:50 PM | 2021-infrastructure-stable |

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| 3196 | GROMACS | Bug | New | Normal | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing | | 11/01/2019 11:28 PM | |
| 3166 | GROMACS | Bug | New | Normal | Compilation failing on Ubuntu 19.04 with Cuda 10.1 | | 10/19/2019 09:13 PM | |
| 3165 | GROMACS | Bug | New | Normal | task assignment silent abort | | 10/18/2019 07:46 PM | |
| 3150 | GROMACS | Bug | New | Normal | gmxapi data type annotations are confusing and inadequate | Eric Irrgang | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3141 | GROMACS | Bug | New | Normal | gmxapi File placeholders missing from beta release | Eric Irrgang | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3136 | GROMACS | Bug | New | Normal | gmxapi.operation data flow topology unclear or incomplete | Eric Irrgang | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 3127 | GROMACS | Bug | New | Normal | mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia | | 10/09/2019 05:33 PM | |
| 3125 | GROMACS | Bug | Resolved | Normal | OpenCL on Volta and Turing broken | | 02/27/2020 11:01 AM | 2020.2 |
| 3124 | GROMACS | Bug | New | Normal | significant performance loss due to DLB auto-off when PP/PME load >1 | | 01/28/2020 02:44 PM | 2021 |
| 3116 | GROMACS | Bug | New | Normal | regressiontests/freeenergy core dumps on ppc64le | Paul Bauer | 10/04/2019 10:52 PM | |
| 3113 | GROMACS | Bug | New | Low | Use of read_tps_conf is deprecated | Paul Bauer | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 3101 | GROMACS | Bug | Blocked, need info | Normal | detect compilation failed | Erik Lindahl | 12/27/2019 10:52 AM | |
| 3088 | GROMACS | Bug | New | Normal | Reference to theory needed for cylindrical pull geometry | | 09/13/2019 11:26 AM | |
| 3086 | GROMACS | Bug | New | Normal | gmxapi fails with MPI build of GROMACS 2020 | | 09/25/2019 04:18 PM | |
| 3083 | GROMACS | Bug | New | Normal | Listed forces tests failing on ICC19 with AVX2_256 nightly build | | 09/10/2019 11:56 AM | |
| 3075 | GROMACS | Bug | New | Normal | Frozen atoms are moving | Erik Lindahl | 12/27/2019 10:51 AM | |
| 3073 | GROMACS | Bug | New | Normal | Total potential energy goes crazy, but I don't know why this happens. | | 09/04/2019 07:25 PM | |
| 3071 | GROMACS | Bug | Accepted | Normal | complex.nbnxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions | Szilárd Páll | 02/25/2020 03:39 PM | 2020.2 |
| 3068 | GROMACS | Bug | New | Normal | Misleading warning on rerun | | 08/26/2019 03:44 PM | |
| 3066 | GROMACS | Bug | New | Normal | Gauss transform and density fit classes should operate on real values instead of float | Christian Blau | 08/26/2019 11:53 AM | |
| 3058 | GROMACS | Bug | Feedback wanted | Normal | Error when using a large PME grid on a GPU | | 09/04/2019 07:26 PM | |
| 3055 | GROMACS | Bug | Feedback wanted | Normal | Error in gmx xpm2ps | | 08/22/2019 03:27 PM | |
| 3054 | GROMACS | Bug | New | Normal | Missing dihedral define | | 08/02/2019 05:47 PM | |
| 3050 | GROMACS | Bug | New | Low | Fix tests on Solaris | Vedran Miletic | 02/27/2020 11:05 AM | 2020.2 |
| 3049 | GROMACS | Bug | New | Low | gmx nmeig should plot a real infrared spectrum | David van der Spoel | 09/24/2019 03:25 PM | future |
| 3048 | GROMACS | Bug | New | Normal | Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5 | | 07/29/2019 10:41 AM | |

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| 3042 | GROMACS | Bug | New | Normal | core dump error in grompp command | | 10/09/2019 07:30 PM | |
| 3028 | GROMACS | Bug | Feedback wanted | Normal | install fail on Centos 6 | | 07/15/2019 12:32 PM | |
| 3000 | GROMACS | Bug | New | Normal | CMake "webpage" target does not fail when it should | | 06/25/2019 02:43 PM | |
| 2987 | GROMACS | Bug | New | Normal | assess the bonded GPU task assignment default | | 12/20/2019 01:06 PM | 2021 |
| 2981 | GROMACS | Bug | New | Normal | segfault in opencl build | | 06/18/2019 03:30 AM | |
| 2980 | GROMACS | Bug | New | Normal | taskassignment fails with unit tests when GPUs and custom number of ranks is used | | 06/17/2019 05:28 PM | |
| 2978 | GROMACS | Bug | New | Normal | Some suggestions about the gmx current tool | | 06/13/2019 12:41 PM | |
| 2974 | GROMACS | Bug | New | Normal | position-restraints regressiontest fails on intel GPU with OpenCL | | 02/25/2020 03:52 PM | 2020.2 |
| 2958 | GROMACS | Bug | New | Normal | Compiling master (to become 2020) using CUDA 9.0 | | 03/02/2020 03:57 PM | 2020.2 |
| 2954 | GROMACS | Bug | New | Normal | genion changes residue numbering | | 05/26/2019 12:08 AM | |
| 2949 | GROMACS | Bug | New | Normal | cmake fails when building mdrun only | | 07/08/2019 10:04 AM | |
| 2948 | GROMACS | Bug | New | Normal | SIMD support detected as none on AMD R5 2500U | | 05/21/2019 12:58 PM | |
| 2924 | GROMACS | Bug | New | Normal | Failing version check when reading new tpr file with older gromacs version | | 04/12/2019 10:52 AM | |
| 2907 | GROMACS | Bug | New | Normal | Gromacs autocompletion appears to be broken with ZSH | | 07/16/2019 04:46 AM | |
| 2902 | GROMACS | Bug | New | Normal | 2019.1 equilibration issue? (Intel 2018u3) | | 04/30/2019 08:17 AM | |
| 2897 | GROMACS | Bug | New | Normal | rotation/flex2 can still fail on cpu-only run on OpenCL build | | 04/04/2019 06:24 PM | |
| 2883 | GROMACS | Bug | New | Normal | essentialdynamics fail with Intel MPI | | 03/08/2019 03:10 AM | |
| 2876 | GROMACS | Bug | New | Normal | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3) | Erik Lindahl | 03/08/2019 10:32 AM | |
| 2873 | GROMACS | Bug | New | Normal | Simple way to get last frame from trajectory | | 02/28/2019 11:14 PM | |
| 2872 | GROMACS | Bug | New | Normal | gmx solvate and genion topology update | | 02/27/2019 10:18 AM | |
| 2870 | GROMACS | Bug | New | Normal | GPU detection error message missing from the output | | 03/05/2019 03:55 PM | |
| 2869 | GROMACS | Bug | New | Normal | GPU detection error only issued as a note to the log | | 03/05/2019 04:09 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 | |
| 2852 | GROMACS | Bug | New | Low | the in-tree regressiontest download can get out of sync with code | | 01/30/2019 03:58 PM | |
| 2848 | GROMACS | Bug | New | Normal | gmx make_ndx ignores last residue in case only CA's are present in GRO file | | 01/30/2019 06:16 AM | |
| 2832 | GROMACS | Bug | New | Low | PaddedVector move operations broken | Mark Abraham | 12/28/2019 10:40 AM | 2021 |
| 2828 | GROMACS | Bug | Feedback wanted | Normal | Installation issue on Power 9 system with SIMD support | | 01/18/2019 11:54 AM | |
| 2788 | GROMACS | Bug | New | Normal | PME will not run on AMD GPU with NVidia GPU present | | 01/03/2019 02:24 PM | |

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|------|---------|---------|--------------------|----------|---|----------------|---------------------|----------------|
| 2785 | GROMACS | Bug | New | Normal | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG | | 11/30/2018 02:36 PM | |
| 2763 | GROMACS | Bug | New | Normal | GMXAPI layout / grouping in development docs "modules" page | | 12/14/2018 12:49 PM | future |
| 2762 | GROMACS | Bug | Blocked, need info | Normal | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads | | 07/01/2019 11:26 PM | |
| 2754 | GROMACS | Bug | New | Normal | Simulated Tempering seems to be broken | Michael Shirts | 02/05/2019 03:58 PM | |
| 2740 | GROMACS | Bug | New | Normal | mdrun reports incorrect error with -bonded gpu without gpu | Mark Abraham | 11/07/2018 01:59 PM | |
| 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 timesout on i686 and armv7hl with OpenMPI 2.1.5 | Paul Bauer | 01/17/2020 08:40 AM | |
| 2707 | GROMACS | Bug | New | Normal | Installed OpenCL files include clh file from gpu_utils directory | | 10/30/2018 04:02 AM | |
| 2702 | GROMACS | Bug | Accepted | Normal | PME gather reduction race in OpenCL (and CUDA) | | 03/28/2019 03:14 PM | |
| 2693 | GROMACS | Bug | New | Normal | Several memory leaks in mdrun | | 12/18/2018 04:22 AM | future |
| 2657 | GROMACS | Bug | New | Normal | Biphasic tutorial | | 09/28/2018 10:02 AM | |
| 2649 | GROMACS | Bug | New | Normal | Virial calculation necessary for correct energy calculation on GPU | | 12/17/2018 02:32 PM | future |
| 2645 | GROMACS | Bug | New | Normal | Security | | 09/28/2018 01:16 PM | |
| 2637 | GROMACS | Bug | New | High | gmx solvate tears apart molecules | | 09/11/2018 07:43 PM | |
| 2628 | GROMACS | Bug | Resolved | Normal | GMXRC removes trailing colon from existing MANPATH | | 11/02/2020 11:45 AM | |
| 2624 | GROMACS | Bug | New | Normal | GPU build system not robust enough | | 09/05/2018 02:00 AM | |
| 2611 | GROMACS | Bug | New | Normal | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX | | 08/14/2018 07:03 PM | |
| 2607 | GROMACS | Bug | New | Normal | Grompp becomes extremely slow when many pull groups are present | | 08/11/2018 08:54 AM | |
| 2606 | GROMACS | Bug | New | Normal | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert | | 08/10/2018 01:48 AM | |
| 2602 | GROMACS | Bug | New | Low | build information gets outdated if build tree is reused | | 08/13/2018 09:04 PM | |
| 2600 | GROMACS | Bug | New | High | coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype | | 08/07/2018 06:50 PM | |
| 2598 | GROMACS | Bug | New | Normal | Tools using read_next_x cannot read TNG files with sanitizers | | 10/15/2018 01:16 PM | future |
| 2582 | GROMACS | Bug | Blocked, need info | Normal | Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6 | Szilárd Páll | 07/23/2018 07:46 PM | |
| 2580 | GROMACS | Bug | Feedback wanted | High | sc-coul option yields different free energy estimate on a ligand with zero partial charge | | 09/11/2018 08:10 AM | |
| 2576 | GROMACS | Bug | New | Normal | gmx potential -correct outputs the wrong potential | | 07/25/2018 02:58 PM | |
| 2573 | GROMACS | Bug | New | High | Different mdp files describing the same change yield different free energy on the same trajectory | | 07/19/2018 06:52 PM | |

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| 2568 | GROMACS | Bug | New | Low | gmx editconf -rotate does not rotate the box | | 07/10/2018 10:27 AM | future |
| 2567 | GROMACS | Bug | New | Normal | make check fails at test 23 SIMD errors | | 07/10/2018 09:35 AM | |
| 2564 | GROMACS | Bug | New | Normal | Result Summary Different For Jobs With Different Numbers of Nodes | | 07/05/2018 02:39 PM | |
| 2563 | GROMACS | Bug | New | Normal | Windows 7 Compilation with GPU support | | 07/02/2018 09:58 AM | |
| 2555 | GROMACS | Bug | New | Low | building GROMACS 2018.2 | | 07/03/2018 11:41 PM | |
| 2544 | GROMACS | Bug | New | Normal | gmx rmsf does not fix periodicity in reference structure | David van der Spoel | 08/21/2018 10:36 AM | future |
| 2526 | GROMACS | Bug | New | Normal | Bug of gmx hbond | | 05/30/2018 03:12 PM | |
| 2513 | GROMACS | Bug | Feedback wanted | Normal | ref_t and temperature incorrect with coulomb-type = user | Yu Du | 05/31/2018 04:05 PM | |
| 2483 | GROMACS | Bug | New | Low | gmx dump writes mdp files that can not be parsed by grompp | Paul Bauer | 10/08/2018 10:50 AM | future |
| 2482 | GROMACS | Bug | Feedback wanted | Normal | Atoms/molecules in freezegrps move and system crashes | | 05/18/2018 07:13 PM | |
| 2480 | GROMACS | Bug | New | Normal | pdb2gmx does not protonate correctly for united-atom Gromos | Mark Abraham | 12/20/2019 12:17 PM | 2021 |
| 2473 | GROMACS | Bug | New | Normal | mdrun sometimes stalls due to large coordinates with no constraints | | 04/04/2018 10:15 PM | |
| 2468 | GROMACS | Bug | New | Low | incorrect GPU timing reported with OpenCL and domain decomposition | | 12/17/2018 01:28 PM | future |
| 2460 | GROMACS | Bug | New | Normal | Allow inclusion of user libraries through CMake cache variables | | 03/28/2018 08:47 PM | |
| 2427 | GROMACS | Bug | New | Normal | gmx select gives syntax error for selection involving evaluating simple arithmetic expression | | 02/27/2018 05:15 PM | |
| 2393 | GROMACS | Bug | New | Normal | incorrect error message with omitted command line flag before its argument | | 01/24/2018 11:24 PM | |
| 2390 | GROMACS | Bug | Feedback wanted | Normal | GROMACS build system should check for valid nvcc flags before use | | 12/20/2019 12:13 PM | 2021 |
| 2380 | GROMACS | Bug | New | Low | cycle counter issues with separate PME rank + GPUs | | 01/16/2018 10:21 PM | |
| 2373 | GROMACS | Bug | New | Low | gmx -nice can't work | | 01/04/2018 11:17 AM | |
| 2360 | GROMACS | Bug | New | Low | error at counter reset with PME-only rank | | 01/05/2018 12:43 PM | future |
| 2255 | GROMACS | Bug | New | Normal | nstlist override stopped affecting the input parameter listing | | 12/17/2017 08:05 AM | |
| 2252 | GROMACS | Bug | New | Low | Memory allocation failures with large page sizes during PME tuning | | 12/14/2017 04:27 AM | |
| 2241 | GROMACS | Bug | New | Low | refdata can segfault when reading | | 09/07/2017 11:57 AM | |
| 2233 | GROMACS | Bug | Accepted | Normal | replica exchange and -append bugged? | | 03/05/2018 01:38 PM | |
| 2232 | GROMACS | Bug | New | Normal | pdb2gmx can't form special bonds with terminal patched atoms | | 12/03/2017 01:35 PM | |
| 2231 | GROMACS | Bug | New | Normal | convert-tpz aborts when saving subset of the system | | 01/12/2018 03:52 PM | |
| 2217 | GROMACS | Bug | New | Low | GPU emulation and separate PME ranks doesn't work properly | | 12/12/2017 11:50 AM | |

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| 2211 | GROMACS | Bug | New | Low | gmx writes normal output to stderr | | 03/05/2018 02:00 PM | future |
| 2208 | GROMACS | Bug | New | Normal | cuFFT linking | | 06/30/2017 01:58 PM | |
| 2192 | GROMACS | Bug | Accepted | Low | grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error | Berk Hess | 12/20/2019 12:11 PM | 2021 |
| 2147 | GROMACS | Bug | Feedback wanted | Normal | Parrinello-Rahman barostat not properly working | | 06/06/2017 07:53 AM | |
| 2113 | GROMACS | Bug | New | Normal | Google tests and execution order | | 03/05/2018 02:05 PM | |
| 2094 | GROMACS | Bug | New | Normal | Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size | | 01/20/2017 04:56 PM | |
| 2065 | GROMACS | Bug | New | Normal | thread-MPI internal errors | | 11/08/2018 03:43 PM | |
| 2052 | GROMACS | Bug | New | Low | trjconv does not recognize periodic molecules | David van der Spoel | 01/12/2018 11:05 AM | |
| 2039 | GROMACS | Bug | New | Normal | mdrun -pinstride defaults are too confusing | | 12/13/2017 04:14 AM | |
| 2020 | GROMACS | Bug | New | Normal | Possible issue with md-vv integrator | Mark Abraham | 03/11/2017 08:30 AM | |
| 1985 | GROMACS | Bug | Fix uploaded | Low | CUDA build system refactoring awaiting review | | 12/20/2019 12:07 PM | 2021 |
| 1934 | GROMACS | Bug | New | Normal | QMMM with ORCA: memory leaks, buffer overflows and much more | | 07/10/2016 09:26 AM | |
| 1919 | GROMACS | Bug | Accepted | Normal | static linking issues cause by hwloc support | | 10/12/2018 10:49 PM | future |
| 1880 | GROMACS | Bug | Feedback wanted | Normal | PP-PME load balancing issue | Berk Hess | 10/03/2018 09:45 PM | future |
| 1843 | GROMACS | Bug | In Progress | Normal | pbx=xy with 2 walls floating point exception with the verlet scheme | Berk Hess | 10/31/2016 11:35 AM | |
| 1839 | GROMACS | Bug | Accepted | Low | pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx | | 07/09/2016 07:27 PM | future |
| 1827 | GROMACS | Bug | New | Low | cmake multi-configuration generator support partly broken | | 12/11/2017 05:20 PM | future |
| 1811 | GROMACS | Bug | New | Normal | Extrae build issues | | 12/13/2017 03:43 AM | |
| 1770 | GROMACS | Bug | New | Normal | segmentation fault with free energy changes and multiple GPU's | | 07/14/2015 03:24 AM | |
| 1730 | GROMACS | Bug | New | Normal | gmx compare does not compare all fields of a .tpr | | 06/12/2015 09:33 PM | future |
| 1667 | GROMACS | Bug | New | Normal | gmx convert-tpr writes wrong number of mol in output tpr | David van der Spoel | 06/27/2016 08:29 PM | |
| 1655 | GROMACS | Bug | New | Normal | g_membed and box type | | 12/09/2014 01:33 PM | |
| 1648 | GROMACS | Bug | Feedback wanted | Normal | Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges | Michael Shirts | 06/25/2015 06:07 AM | |
| 1618 | GROMACS | Bug | In Progress | Normal | g_protonate segfaults unconditionally | Erik Lindahl | 08/17/2015 02:10 PM | |
| 1583 | GROMACS | Bug | New | Normal | gmx msd with mol flag requires excessive memory | | 12/18/2017 03:34 PM | |
| 1568 | GROMACS | Bug | New | Low | inconsistent/incorrect threading checks and reporting in mdrun | | 05/25/2016 02:01 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 1481 | GROMACS | Bug | New | Low | g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files | David van der Spoel | 06/12/2014 01:37 PM | |
| 1476 | GROMACS | Bug | New | Low | Odd behavior with verlet-buffer-drift | | 05/25/2016 01:45 AM | future |
| 1448 | GROMACS | Bug | New | Normal | multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing) | Mark Abraham | 06/23/2016 03:15 PM | |
| 1442 | GROMACS | Bug | Feedback wanted | Normal | Not consistent solvation free energies differences | Michael Shirts | 07/11/2016 08:13 PM | |
| 1354 | GROMACS | Bug | New | Normal | Constant acceleration NEMD is broken. | David van der Spoel | 01/09/2019 04:42 PM | |
| 1339 | GROMACS | Bug | New | Normal | Center of mass drift with Nose-Hoover, MTTK and md-vv | Michael Shirts | 06/18/2015 08:53 PM | future |
| 1235 | GROMACS | Bug | New | Normal | peptide dihedral angle definitions violate IUPAC | David van der Spoel | 06/19/2015 12:24 AM | future |
| 1190 | GROMACS | Bug | New | Normal | Use of FORCE in setting cached variables | Mark Abraham | 06/17/2014 06:09 AM | |
| 1166 | GROMACS | Bug | New | Low | g_order is incorrect for unsaturated carbons | David van der Spoel | 02/06/2020 02:32 PM | future |
| 3439 | GROMACS | Feature | New | Normal | Optimize successive simulation segments | | 03/11/2020 01:42 PM | |
| 3436 | GROMACS | Feature | New | Normal | Implement AWH for modular simulator | Pascal Merz | 03/11/2020 06:32 AM | 2021-infrastructure-stable |
| 3435 | GROMACS | Feature | New | Normal | Implement pull for modular simulator | Pascal Merz | 03/11/2020 06:31 AM | 2021-infrastructure-stable |
| 3434 | GROMACS | Feature | New | Normal | Support box deformation in modular simulator | Pascal Merz | 03/11/2020 12:50 AM | 2021-infrastructure-stable |
| 3433 | GROMACS | Feature | New | Normal | Decide how to handle multisim with modular simulator | Pascal Merz | 03/11/2020 06:42 AM | 2021-infrastructure-stable |
| 3432 | GROMACS | Feature | New | Normal | Implement essential dynamics for modular simulator | Pascal Merz | 03/11/2020 12:38 AM | 2021-infrastructure-stable |
| 3431 | GROMACS | Feature | New | Normal | Implement virtual sites for modular simulator | Pascal Merz | 03/11/2020 12:33 AM | 2021-infrastructure-stable |
| 3430 | GROMACS | Feature | New | Normal | Implement NMR restraints for modular simulator | Pascal Merz | 03/11/2020 12:28 AM | 2021-infrastructure-stable |
| 3428 | GROMACS | Feature | New | Normal | Implement SIMD version of modular simulator propagators | Pascal Merz | 03/11/2020 12:12 AM | 2021-infrastructure-stable |
| 3427 | GROMACS | Feature | New | Normal | Support freeze groups in modular simulator | Pascal Merz | 03/11/2020 12:07 AM | 2021-infrastructure-stable |
| 3426 | GROMACS | Feature | New | Normal | Support acceleration in modular simulator | Pascal Merz | 03/11/2020 04:09 PM | 2021-infrastructure-stable |
| 3425 | GROMACS | Feature | New | Normal | Implement rerun for the modular simulator | Pascal Merz | 03/10/2020 11:57 PM | 2021-infrastructure-stable |
| 3424 | GROMACS | Feature | New | Normal | Implement stochastic dynamics / langevin integrator in modular simulator | Pascal Merz | 03/10/2020 11:48 PM | 2021-infrastructure-stable |
| 3423 | GROMACS | Feature | New | Normal | Implement additional temperature and pressure control algorithms for modular simulator | Pascal Merz | 03/10/2020 11:22 PM | 2021-infrastructure-stable |
| 3417 | GROMACS | Feature | New | Normal | Make modular simulator feature-complete | Pascal Merz | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3410 | GROMACS | Feature | New | Normal | Random Acceleration Molecular Dynamics (RAMD) | Bernd Doser | 03/05/2020 03:22 PM | 2021 |
| 3402 | GROMACS | Feature | New | Normal | Clarify distinction between public API documentation and developer docs. | | 02/26/2020 04:16 PM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|------------------|---------------------|----------------------------|
| 3401 | GROMACS | Feature | New | Normal | Policy and procedure for installed headers (public API) | | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3395 | GROMACS | Feature | Feedback wanted | Normal | Consider scripted composition of Dockerfiles | | 03/16/2020 12:16 PM | |
| 3394 | GROMACS | Feature | New | Normal | improve gmxapi error handling | Eric Irrgang | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3393 | GROMACS | Feature | Resolved | Normal | Allow gmxapi.commandline_operation to use STDIN | Eric Irrgang | 02/25/2020 05:15 PM | 2021-infrastructure-stable |
| 3379 | GROMACS | Feature | New | Normal | C++ API for simulation input and output | | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3378 | GROMACS | Feature | New | Normal | genion usage without stdin (facilitates use in gmx python api) | | 02/13/2020 12:04 PM | |
| 3374 | GROMACS | Feature | New | Normal | SimulationInput abstraction | | 03/03/2020 05:32 PM | 2021-refactoring |
| 3371 | GROMACS | Feature | New | Normal | Control FEP using AWH | Magnus Lundborg | 02/06/2020 02:20 PM | 2021 |
| 3369 | GROMACS | Feature | New | Normal | Add quote about "the truth" | | 02/05/2020 05:08 PM | |
| 3363 | GROMACS | Feature | New | Normal | Improve FEP testing | Pascal Merz | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3362 | GROMACS | Feature | New | Normal | gmx traj: add an option to plot each component in a separate file | | 01/29/2020 06:18 PM | |
| 3355 | GROMACS | Feature | Accepted | Normal | New PME parallel (GPU) scheme | Jonathan Vincent | 02/12/2020 11:58 AM | |
| 3352 | GROMACS | Feature | New | Normal | GPU update-constraints feature support | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3351 | GROMACS | Feature | New | Normal | GPU update-constraints code organization and integration | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3350 | GROMACS | Feature | New | Normal | GPU update-constraints performance | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3332 | GROMACS | Feature | New | Normal | gmx helixorient doesn't have a -tu option to change time unit | | 01/22/2020 11:57 AM | |
| 3328 | GROMACS | Feature | New | Normal | Testing framework for task assignment | | 01/22/2020 09:48 AM | 2021-refactoring |
| 3318 | GROMACS | Feature | In Progress | Normal | Use wrappers for the GPU buffer copy/allocations | Artem Zhmurov | 01/23/2020 12:01 PM | 2021-refactoring |
| 3313 | GROMACS | Feature | Accepted | Normal | Introduce and use opaque types for the DeviceStream and DeviceContext | Artem Zhmurov | 01/23/2020 12:00 PM | 2021-refactoring |
| 3311 | GROMACS | Feature | In Progress | Normal | GPU infrastructure development | | 03/20/2020 09:54 AM | 2021-refactoring |
| 3307 | GROMACS | Feature | New | Normal | General interface for communication between simulation ranks | | 01/22/2020 03:22 PM | 2021-refactoring |
| 3298 | GROMACS | Feature | New | Normal | start early PP work for first dimension of halo exchange | | 03/01/2020 01:36 PM | |
| 3295 | GROMACS | Feature | New | Normal | Expand gmxapi.modify_input use cases. | Eric Irrgang | 01/16/2020 05:13 PM | 2021-refactoring |
| 3288 | GROMACS | Feature | New | Normal | Use build system infrastructure instead of custom scripts to manage API levels. | | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3285 | GROMACS | Feature | Resolved | Normal | Run simulations from the same tpr file with different random seeds | | 02/27/2020 11:22 PM | future |
| 3283 | GROMACS | Feature | Resolved | Normal | Support for the string method with swarms of trajectories in GROMACS | | 03/01/2020 01:16 PM | 2021 |
| 3277 | GROMACS | Feature | New | Normal | Allow testing feature that is partly implemented | | 12/31/2019 12:44 PM | 2021 |
| 3242 | GROMACS | Feature | New | Normal | Please do not remove the -nsteps flag | | 03/01/2020 01:59 PM | |
| 3179 | GROMACS | Feature | New | Normal | Clarify access to parallel data outputs | Eric Irrgang | 10/26/2019 12:23 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|-----------------|---------------------|----------------------------|
| 3177 | GROMACS | Feature | New | Normal | Spack package management support | | 11/06/2019 06:37 PM | |
| 3172 | GROMACS | Feature | New | Normal | QM/MM Interface with CP2K | Dmitry Morozov | 01/17/2020 12:18 PM | future |
| 3160 | GROMACS | Feature | Fix uploaded | High | implement direct comm for different src/target memory spaces | Alan Gray | 02/14/2020 11:28 AM | 2021-infrastructure-stable |
| 3152 | GROMACS | Feature | New | Normal | Infrastructure and patterns for expressing public interfaces | | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3149 | GROMACS | Feature | New | Normal | Python user interface for obtaining simulation artifacts as files. | Eric Irrgang | 10/15/2019 06:21 PM | |
| 3148 | GROMACS | Feature | New | Normal | Roadmap for gmxapi filesystem interactions. | Eric Irrgang | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3147 | GROMACS | Feature | New | Normal | gmxapi workflow checkpointing | Eric Irrgang | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3140 | GROMACS | Feature | New | Normal | Allow explicit input definition for gmxapi.operation function wrapper | Eric Irrgang | 12/10/2019 02:00 PM | 2021-infrastructure-stable |
| 3138 | GROMACS | Feature | New | Normal | Improve ensemble support in Context specification. | | 10/15/2019 03:56 PM | |
| 3135 | GROMACS | Feature | New | Normal | Make GPU traits ino opaque types | | 10/14/2019 10:24 AM | |
| 3134 | GROMACS | Feature | Feedback wanted | Normal | gmxapi Python exception names may need improvement | Eric Irrgang | 10/13/2019 01:50 PM | |
| 3126 | GROMACS | Feature | New | Normal | State propagator GPU data manager | | 10/09/2019 02:42 PM | |
| 3117 | GROMACS | Feature | New | Normal | Coulomb FEP PME on GPU | Magnus Lundborg | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 3115 | GROMACS | Feature | New | Normal | Device stream manager | | 10/04/2019 09:00 AM | |
| 3114 | GROMACS | Feature | New | Normal | Improve GPU update-constraints module | Artem Zhmurov | 02/10/2020 04:30 PM | 2021 |
| 3069 | GROMACS | Feature | New | Low | Iterator over span and indices into this span (zip-style iterator) | Christian Blau | 08/29/2019 11:11 AM | future |
| 3045 | GROMACS | Feature | New | Low | Option to remove v-sites in trjconv? | | 07/19/2019 04:42 PM | |
| 3038 | GROMACS | Feature | New | Normal | Improvements to MD plugin development environment | Eric Irrgang | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 3032 | GROMACS | Feature | Feedback wanted | Normal | Clean up dev-manual structure | | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3030 | GROMACS | Feature | New | Normal | RST style guidelines | | 07/09/2019 03:38 PM | |
| 3021 | GROMACS | Feature | Feedback wanted | Normal | Completion of docs for GPU developments | | 03/02/2020 03:58 PM | 2020.2 |
| 3020 | GROMACS | Feature | New | Low | modernize DeviceBuffer and GPU memory management | | 08/13/2019 06:01 PM | |
| 2996 | GROMACS | Feature | In Progress | Normal | gmxapi execution model | Eric Irrgang | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 2994 | GROMACS | Feature | New | Normal | Data flow topology in gmxapi 2020 | | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 2993 | GROMACS | Feature | New | Normal | Scalar and structured type expression and definitions for API | Eric Irrgang | 10/17/2019 09:55 AM | |
| 2984 | GROMACS | Feature | New | Normal | More Extensive Selections Examples | Dallas Warren | 06/18/2019 11:50 PM | |
| 2977 | GROMACS | Feature | New | Normal | print DD load balancing improvement | | 06/13/2019 10:56 AM | |
| 2975 | GROMACS | Feature | New | Normal | LJ PME calculations on GPUs | | 06/12/2019 01:17 PM | |
| 2967 | GROMACS | Feature | New | Normal | GPU reallocateDeviceBuffer improvements | | 01/23/2020 12:15 PM | 2021-refactoring |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|------------------|
| 2961 | GROMACS | Feature | New | Normal | How should Python package find GROMACS resources under various circumstances? | | 12/09/2019 10:47 AM | |
| 2956 | GROMACS | Feature | New | Normal | SAXS resolution | | 05/17/2019 09:58 AM | |
| 2944 | GROMACS | Feature | New | Normal | Roadmap for thermostats / barostats in new propagation/integration scheme | Michael Shirts | 12/27/2019 04:00 PM | 2021 |
| 2931 | GROMACS | Feature | New | Normal | Tables in Verlet kernels | | 04/29/2019 12:01 PM | |
| 2930 | GROMACS | Feature | New | Normal | Limited range for reference group detection in cylinder pulling | | 04/26/2019 05:17 PM | |
| 2928 | GROMACS | Feature | New | Normal | Add ability to use expression "count of ATOM_EXPR" in selection statements. | | 04/16/2019 04:52 PM | |
| 2915 | GROMACS | Feature | In Progress | High | GPU direct communications | | 02/14/2020 12:48 PM | |
| 2910 | GROMACS | Feature | New | Normal | Mixed scaling for 1-4 interactions | | 04/10/2019 10:13 PM | |
| 2896 | GROMACS | Feature | Feedback wanted | Normal | Python packaging | | 01/16/2020 07:11 PM | 2021-refactoring |
| 2891 | GROMACS | Feature | In Progress | Normal | PME/PP GPU communications | | 02/14/2020 12:40 PM | |
| 2890 | GROMACS | Feature | In Progress | Normal | GPU Halo Exchange | | 02/14/2020 12:41 PM | 2021 |
| 2866 | GROMACS | Feature | New | Normal | Alternative non-bonded potentials | David van der Spoel | 03/05/2019 03:50 PM | future |
| 2860 | GROMACS | Feature | New | Normal | Option for outputting min/max coordinates in gmx traj | | 02/08/2019 12:35 AM | |
| 2846 | GROMACS | Feature | New | Low | Set rpath in FindLibStdCpp.cmake | | 02/02/2019 08:09 AM | |
| 2840 | GROMACS | Feature | New | Normal | Test that functionality does not compile that is not supposed to. | | 01/25/2019 02:35 PM | future |
| 2806 | GROMACS | Feature | New | Normal | SIMD algorithms for ARM SVE // nobonded cluster and others | | 12/27/2019 03:59 PM | 2021 |
| 2791 | GROMACS | Feature | In Progress | Normal | Implement a module for lambda-dynamics simulations (lambda_site module) | Thomas Ullmann | 03/01/2019 01:36 AM | future |
| 2774 | GROMACS | Feature | New | Normal | Refactor shell code into its own integrator | David van der Spoel | 12/27/2019 04:05 PM | 2021 |
| 2761 | GROMACS | Feature | New | Low | lincs-order 4 is too conservative for some force fields | | 11/16/2018 09:55 AM | |
| 2755 | GROMACS | Feature | New | Low | md5 sums and sha256, sha512 hashes | Benson Muite | 02/19/2019 11:00 PM | |
| 2739 | GROMACS | Feature | New | Normal | Parallel continuous tempering and enhanced sampling feature | | 11/13/2018 11:36 PM | |
| 2715 | GROMACS | Feature | New | Normal | Avoid requesting the user to recompile gromacs for Intel OpenCL support | | 12/27/2019 04:06 PM | future |
| 2713 | GROMACS | Feature | New | Normal | Constant offset for external electric fields | | 10/28/2018 12:57 AM | |
| 2710 | GROMACS | Feature | New | Normal | Separate dvdI for each molecule (of couple-moltype) when running FEP | | 12/27/2019 04:41 PM | 2021 |
| 2667 | GROMACS | Feature | New | Normal | Suggested steps for calculating entropy in solution and binding | David van der Spoel | 03/01/2020 01:35 PM | 2020.2 |
| 2643 | GROMACS | Feature | New | Low | mdp options and/or docs for anisotropic aspects of implementations | | 09/12/2018 02:23 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|--|---------------------|---------------------|----------------|
| 2622 | GROMACS | Feature | New | Low | Reduce severity of Berendsen warning | | 08/23/2018 11:16 PM | future |
| 2601 | GROMACS | Feature | New | Normal | Free energy calculations, soft-core potential | Vytautas Gapsys | 02/10/2020 11:29 AM | future |
| 2596 | GROMACS | Feature | New | Normal | Constant potential method | Benson Muite | 05/10/2019 09:54 AM | |
| 2594 | GROMACS | Feature | New | Normal | Multi-level GMX API | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2587 | GROMACS | Feature | In Progress | Normal | Provide Context (e.g. to runner code) to manage client and runtime environment | | 10/15/2018 03:34 PM | |
| 2585 | GROMACS | Feature | Resolved | Normal | Infrastructure supporting external API | | 12/11/2019 12:39 PM | |
| 2581 | GROMACS | Feature | Accepted | Normal | User interface for hybrid Monte Carlo | | 12/20/2019 12:24 PM | future |
| 2579 | GROMACS | Feature | New | Normal | Add dimensionality option to gmx trjconv -center | | 07/19/2018 04:53 PM | future |
| 2574 | GROMACS | Feature | New | Normal | iForceSchedule Abstraction | Prashanth Kanduri | 03/29/2019 05:20 PM | future |
| 2570 | GROMACS | Feature | New | Normal | Better string formatting and printing | | 05/02/2019 12:20 PM | |
| 2556 | GROMACS | Feature | New | Normal | make default selections suitable for DNA and RNA | Mark Abraham | 06/20/2018 01:48 PM | |
| 2547 | GROMACS | Feature | New | Low | Add option of averaging and obtaining error bars for AWH PMFs | Viveca Lindahl | 06/06/2018 11:31 AM | future |
| 2545 | GROMACS | Feature | New | Normal | Should grompp fix periodicity of input files? | David van der Spoel | 10/03/2018 11:32 PM | future |
| 2491 | GROMACS | Feature | New | Low | Allow constant bias AWH simulations | Viveca Lindahl | 06/05/2018 10:38 PM | future |
| 2451 | GROMACS | Feature | Resolved | Normal | Linear virtual sites with fixed distance | David van der Spoel | 09/16/2019 01:15 PM | |
| 2429 | GROMACS | Feature | New | Normal | Add option of periodic chain topology to pdb2gmx | | 03/10/2018 01:01 PM | |
| 2428 | GROMACS | Feature | New | Normal | Add way of selecting interactive arguments of pdb2gmx by string rather than an index | | 02/27/2018 06:28 PM | |
| 2426 | GROMACS | Feature | In Progress | Normal | Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA) | | 10/03/2018 11:31 PM | future |
| 2354 | GROMACS | Feature | New | Normal | develop configuration file support for control of task layout | | 09/19/2018 03:01 PM | future |
| 2310 | GROMACS | Feature | Accepted | Low | Let mdrun dump coordinates with non-finite energy | | 10/03/2018 09:47 PM | future |
| 2289 | GROMACS | Feature | New | Normal | gmx spatial add ability to perform over multiple reference structures | | 11/08/2017 12:31 AM | |
| 2288 | GROMACS | Feature | Accepted | Low | gmx msd doesn't optimally handle missing input trajectory frames | | 11/10/2017 11:03 AM | |
| 2283 | GROMACS | Feature | New | Normal | Force distribution analysis | Bernd Doser | 10/27/2017 11:44 AM | |
| 2282 | GROMACS | Feature | New | Normal | Density map toolset | Christian Blau | 03/21/2019 06:08 PM | future |
| 2254 | GROMACS | Feature | Resolved | Normal | GPU extensions for Google Tests | | 10/06/2020 12:15 PM | |
| 2248 | GROMACS | Feature | New | Normal | Label all SIMD functions as pure/nodiscard | | 02/04/2019 04:49 AM | |
| 2239 | GROMACS | Feature | New | Normal | split libgromacs into base and full | | 01/07/2019 01:47 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------|
| 2229 | GROMACS | Feature | New | High | Full Object Oriented Modularization of GROMACS MDRUN Codebase | Mark Abraham | 08/22/2018 05:03 PM | future |
| 2226 | GROMACS | Feature | New | Normal | Harmonise commands for exit in make_ndx and distance | | 08/04/2017 12:24 PM | |
| 2224 | GROMACS | Feature | New | Normal | Proposed feature: conditional stop | Vedran Miletic | 12/20/2019 12:11 PM | 2021 |
| 2220 | GROMACS | Feature | New | Normal | report relevant env var behaviour to console | | 07/31/2017 09:40 PM | |
| 2218 | GROMACS | Feature | Feedback wanted | Normal | A tiny feature: damping for umbrella pull | | 08/16/2017 07:20 PM | |
| 2207 | GROMACS | Feature | New | Normal | solvent excluded volume of large molecule with periodic boundary condition | | 06/16/2017 10:37 AM | |
| 2194 | GROMACS | Feature | Accepted | Low | xvg output requested as an output option in place of xpm files | | 05/31/2017 04:26 PM | |
| 2186 | GROMACS | Feature | New | Low | Potential change for logical improvements: move control of constraints purely to the .mdp | Michael Shirts | 11/27/2018 11:27 AM | future |
| 2139 | GROMACS | Feature | New | Normal | More precise/explicit documentation conventions | | 01/07/2018 11:54 PM | |
| 2137 | GROMACS | Feature | New | Normal | Preliminary refactoring of constraints and update machinery. | Michael Shirts | 03/11/2017 08:32 AM | future |
| 2132 | GROMACS | Feature | New | Normal | Intermediate code for xvg handling | | 03/08/2017 05:12 PM | future |
| 2126 | GROMACS | Feature | New | Normal | implement native CUDA support in CMake | | 10/29/2019 09:03 PM | |
| 2118 | GROMACS | Feature | New | Low | More verbose comments requested in header of gmx distance -oxyz | | 02/08/2017 05:46 AM | |
| 2111 | GROMACS | Feature | In Progress | Normal | Implement Gaussian screening of electrostatics | | 02/23/2019 12:33 PM | |
| 2101 | GROMACS | Feature | New | Low | warninp could print the offending line, as well as its number | | 01/20/2017 03:06 PM | |
| 2097 | GROMACS | Feature | New | Low | Move output of dhdl file entirely to edr, rather than having a separate text dhdl file | | 01/05/2017 05:21 PM | future |
| 2090 | GROMACS | Feature | New | Normal | redirecting stdout or stderr for testing | Mark Abraham | 12/15/2016 03:15 AM | |
| 2080 | GROMACS | Feature | New | Normal | add grompp warning for suitability for domain decomposition | | 11/23/2016 03:03 PM | |
| 2070 | GROMACS | Feature | In Progress | Normal | Physical validation testing | Michael Shirts | 01/03/2020 09:36 PM | future |
| 2068 | GROMACS | Feature | New | Normal | Access to low level classes | | 03/02/2019 01:37 AM | future |
| 2060 | GROMACS | Feature | New | Normal | Convert enum to enum class | | 10/17/2016 05:27 PM | |
| 2056 | GROMACS | Feature | New | Low | rename "gmx select" | | 10/03/2016 08:24 PM | |
| 2054 | GROMACS | Feature | Accepted | High | PME on GPU | Aleksei lupinov | 12/20/2019 12:18 PM | future |
| 2034 | GROMACS | Feature | New | Normal | Unit tests for bonded forces | David van der Spoel | 06/29/2019 10:22 AM | future |
| 2018 | GROMACS | Feature | New | Normal | Pulling along a line between given points | | 07/27/2016 09:59 AM | |
| 2015 | GROMACS | Feature | New | Normal | Auto recovery from dd communication error | | 07/28/2016 03:17 PM | |
| 2005 | GROMACS | Feature | New | Normal | Full Correlation Analysis (FCA) as Trajectory Analysis Module | Christian Blau | 02/07/2018 02:19 PM | future |
| 2001 | GROMACS | Feature | New | Normal | add MPI info to the mdrun log header | | 07/06/2016 05:21 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|--|------------------------|---------------------|----------------|
| 1994 | GROMACS | Feature | New | Low | explore using JIT for CUDA | | 07/11/2016 10:20 PM | future |
| 1974 | GROMACS | Feature | New | Normal | Report atom numbers and types in the error message about missed parameters | | 05/30/2016 09:24 AM | |
| 1972 | GROMACS | Feature | New | Normal | external potential modules for refinement against experimental data | | 08/22/2018 05:03 PM | future |
| 1966 | GROMACS | Feature | New | Low | Hydrogen mass repartiniog | | 05/25/2016 06:04 PM | future |
| 1964 | GROMACS | Feature | Accepted | Normal | "pull=no" should not produce warnings about "unknown" pull keywords | | 05/20/2016 02:37 PM | |
| 1953 | GROMACS | Feature | New | Low | use more regular polymorphism for GPU code | | 05/06/2016 10:06 PM | future |
| 1948 | GROMACS | Feature | New | Low | add warning when non-identical GPUs are used | | 06/12/2017 08:45 PM | |
| 1902 | GROMACS | Feature | Accepted | Low | Add grompp check that non-excluded atoms are not too close to each other in the starting structure | | 02/15/2016 01:34 PM | |
| 1900 | GROMACS | Feature | New | Normal | Implement some new errors in grompp | | 06/22/2016 05:20 PM | |
| 1885 | GROMACS | Feature | New | Normal | DPD Thermostat | | 01/26/2016 10:17 AM | |
| 1867 | GROMACS | Feature | New | Normal | make coupling implementations reversible | | 12/02/2015 07:43 AM | |
| 1864 | GROMACS | Feature | New | Normal | write tng files with energies | Magnus Lundborg | 07/11/2016 08:00 PM | |
| 1854 | GROMACS | Feature | New | Normal | Remove all cyclic dependencies | | 05/25/2017 08:34 AM | |
| 1849 | GROMACS | Feature | New | Normal | expanded ensemble -- Adaptive Integration Method | Christopher Mirabzadeh | 07/11/2016 08:01 PM | |
| 1842 | GROMACS | Feature | New | Normal | Replace XML with JSON | | 01/18/2018 05:12 PM | |
| 1715 | GROMACS | Feature | New | Low | improve cycle counting GPU sharing and multi-sim | | 08/03/2016 12:32 PM | future |
| 1688 | GROMACS | Feature | New | Low | g_cluster "middle" is not exactly the same as the definition in the cited paper | | 04/01/2015 05:53 AM | |
| 1670 | GROMACS | Feature | New | Normal | create mdrun option checking mini-tool | | 06/23/2016 04:06 PM | |
| 1666 | GROMACS | Feature | New | Normal | new approach for Verlet-scheme kernel generation | Erik Lindahl | 10/08/2018 07:04 PM | future |
| 1665 | GROMACS | Feature | New | Normal | improve free energy non-bonded kernel performance | | 08/26/2019 03:47 PM | future |
| 1658 | GROMACS | Feature | New | Normal | Electrostatics treatment for multiple lambda sites | Berk Hess | 07/11/2016 08:05 PM | |
| 1654 | GROMACS | Feature | New | Normal | How to carry out movement between chemical end states in a multiple end state framework? | Michael Shirts | 07/11/2016 08:05 PM | |
| 1653 | GROMACS | Feature | New | Normal | Decide how to represent multiple lambda states in the .top file and how to parse them | Michael Shirts | 06/05/2018 03:58 PM | |
| 1652 | GROMACS | Feature | New | Normal | Decide how to represent multiple lambda states internally | Michael Shirts | 06/05/2018 03:58 PM | |
| 1641 | GROMACS | Feature | New | Normal | Add toolchain file for Cray systems | | 06/06/2015 11:24 PM | |
| 1635 | GROMACS | Feature | New | Normal | Proper Unicode support | | 06/18/2015 08:34 PM | |
| 1634 | GROMACS | Feature | New | Normal | Boxed Molecular Dynamics | | 11/04/2014 04:40 PM | |
| 1627 | GROMACS | Feature | In Progress | Normal | DPD integrator | | 07/11/2016 08:08 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|--|---------------------|---------------------|----------------|
| 1625 | GROMACS | Feature | New | Normal | Gromacs Python API | | 03/02/2019 01:44 AM | future |
| 1602 | GROMACS | Feature | New | Low | gmx order S per slice along all 3 axes | | 09/22/2014 07:25 AM | |
| 1562 | GROMACS | Feature | New | Normal | introducing a Monte Carlo framework (first application: MC barostat) | Michael Shirts | 07/11/2016 08:08 PM | |
| 1518 | GROMACS | Feature | New | Low | Enable automatic build checking for newer versions | Mark Abraham | 06/04/2014 04:13 PM | future |
| 1511 | GROMACS | Feature | Accepted | Normal | add PDBx (ie mmcif) support | | 10/05/2018 07:14 PM | |
| 1500 | GROMACS | Feature | New | Normal | Post-5.0 feature clean-up plan | Mark Abraham | 08/26/2019 03:47 PM | |
| 1498 | GROMACS | Feature | New | Low | g_dipoles does not work properly with ionic systems | David van der Spoel | 07/11/2016 08:11 PM | |
| 1489 | GROMACS | Feature | New | Normal | Don't solely rely on filename extension | | 04/30/2014 05:23 AM | |
| 1464 | GROMACS | Feature | New | Normal | implement PP-PME re-balancing | Szilárd Páll | 10/16/2015 08:34 AM | future |
| 1437 | GROMACS | Feature | New | Normal | Online help formatting improvements | | 06/04/2015 09:20 PM | future |
| 1422 | GROMACS | Feature | New | Normal | CSH angle incorrect with GROMOS force field and virtual sites | David van der Spoel | 06/12/2014 12:01 AM | |
| 1397 | GROMACS | Feature | New | Normal | gmx eneconv -offset 1.998 -dt 2 is broken for large times | Mark Abraham | 06/12/2014 01:31 AM | future |
| 1377 | GROMACS | Feature | Feedback wanted | Low | Replica exchange if replicas not in ascendent T | David van der Spoel | 06/23/2016 03:48 PM | |
| 1347 | GROMACS | Feature | New | Normal | future of tables | Berk Hess | 01/09/2020 02:37 PM | future |
| 1335 | GROMACS | Feature | New | Normal | Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling | Michael Shirts | 05/13/2014 10:38 AM | future |
| 1332 | GROMACS | Feature | In Progress | Normal | Supporting multiple end states instead of just A and B | Michael Shirts | 06/05/2018 03:58 PM | |
| 1328 | GROMACS | Feature | Accepted | Normal | Names for selection positions | | 07/11/2016 08:15 PM | |
| 1303 | GROMACS | Feature | New | Normal | Adding lambda dependent distance for pull code | Michael Shirts | 07/11/2016 08:18 PM | |
| 1247 | GROMACS | Feature | New | Normal | fix hardcoded references to atom names in analysis tools | Mark Abraham | 06/12/2014 01:20 AM | future |
| 1221 | GROMACS | Feature | Accepted | Normal | More generic position mapping for selections | | 06/10/2014 02:58 PM | future |
| 1192 | GROMACS | Feature | Accepted | Normal | Add support for Verlet scheme with Buckingham | Berk Hess | 07/11/2016 08:19 PM | |
| 1182 | GROMACS | Feature | New | Normal | improve trajectory writing to support parallel I/O | | 05/13/2014 10:42 AM | future |
| 1168 | GROMACS | Feature | In Progress | Low | g_density does not do what users think it does, given PBC over z and constant pressure simulation | Erik Lindahl | 10/20/2018 12:49 AM | future |
| 1167 | GROMACS | Feature | New | Low | trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values | David van der Spoel | 06/23/2014 04:13 AM | future |
| 1165 | GROMACS | Feature | Accepted | Low | Multi-SIMD binaries | | 12/20/2019 12:00 PM | future |
| 1162 | GROMACS | Feature | New | Normal | Implement gb_saltconc | Berk Hess | 02/26/2013 05:33 PM | future |
| 1142 | GROMACS | Feature | New | Low | Synchronizing the differences between point estimation and histogram estimation for free energies | Michael Shirts | 02/20/2014 08:27 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------------|----------|--|------------------|---------------------|----------------------------|
| 1139 | GROMACS | Feature | New | Normal | Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated | | 07/11/2016 08:19 PM | |
| 1137 | GROMACS | Feature | New | Normal | Proposal for integrator framework (do_md) in future GROMACS | Michael Shirts | 02/21/2017 12:48 AM | future |
| 1120 | GROMACS | Feature | New | Low | Make build work with multi-configuration generators | | 06/03/2014 03:04 PM | future |
| 1104 | GROMACS | Feature | New | Low | Implement dihedral restraints | | 02/06/2013 07:04 PM | future |
| 1102 | GROMACS | Feature | New | Normal | Detect incompletely written itp files | | 06/19/2014 03:23 PM | |
| 1083 | GROMACS | Feature | In Progress | Normal | Improve collective error/warning/note handling in mdrun | | 07/11/2016 08:21 PM | |
| 1053 | GROMACS | Feature | In Progress | Normal | L-BFGS doesn't use constraints or call do_em_step | Berk Hess | 01/18/2013 11:00 AM | future |
| 1030 | GROMACS | Feature | Fix uploaded | Low | adding -tu option to some analysis tools | Rossen Apostolov | 07/11/2016 08:22 PM | |
| 1028 | GROMACS | Feature | New | Normal | Tool to calculate fraction of native contacts during simulation | | 11/01/2012 10:27 PM | |
| 1026 | GROMACS | Feature | New | Low | request for gen_vel to work with multiple temperature coupling groups at different temperatures | | 11/17/2016 04:39 PM | |
| 951 | GROMACS | Feature | New | Normal | Multiple versions of Gromacs (e.g., single and double) in the same library/binary | | 01/07/2019 02:10 AM | future |
| 950 | GROMACS | Feature | New | Normal | Path/directory/filename handling in Gromacs | | 07/11/2016 08:24 PM | |
| 921 | GROMACS | Feature | Blocked, need info | Normal | Default index groups and selections | | 07/11/2016 08:27 PM | |
| 907 | GROMACS | Feature | Accepted | Normal | Add tests for verifying installed headers | | 03/11/2014 09:15 PM | future |
| 895 | GROMACS | Feature | In Progress | Normal | g_rmsf previous frame as reference | | 04/29/2013 07:39 PM | future |
| 868 | GROMACS | Feature | In Progress | Normal | Implement parallelization support to analysis framework | Kevin Boyd | 12/20/2019 11:59 AM | 2021 |
| 843 | GROMACS | Feature | New | Low | g_helixorient could benefit from more documentation | Erik Lindahl | 05/23/2014 02:02 PM | |
| 760 | GROMACS | Feature | New | Low | Implement rigid body groups | Berk Hess | 12/30/2012 06:04 AM | future |
| 742 | GROMACS | Feature | New | Normal | Enhancing the performance of the free energy code | | 08/26/2019 04:55 PM | future |
| 731 | GROMACS | Feature | New | Normal | pdb2gmx should warn about missing residues when bonds are too long | | 06/22/2014 10:55 AM | |
| 720 | GROMACS | Feature | Accepted | Low | permit pdb2gmx to choose a kind of HIS based on proton position | | 11/17/2016 03:51 PM | future |
| 438 | GROMACS | Feature | In Progress | Low | New tool: g_correl | Alexey Shvetsov | 06/20/2014 10:38 AM | future |
| 3446 | GROMACS | Task | New | Normal | apply maintainability updates across all GPU kernels | Jonathan Vincent | 03/19/2020 03:31 PM | |
| 3445 | GROMACS | Task | New | Normal | create heuristic for c_skipNeutralAtoms | Jonathan Vincent | 03/17/2020 12:12 PM | |
| 3437 | GROMACS | Task | New | Normal | Use builders to prepare modules | Pascal Merz | 03/11/2020 07:05 AM | 2021-infrastructure-stable |
| 3422 | GROMACS | Task | Resolved | Normal | Implement modular checkpointing for modular simulator | Pascal Merz | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 3421 | GROMACS | Task | New | Normal | Implement client system for global reduction | Pascal Merz | 03/11/2020 03:31 PM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|----------|----------|--|---------------|---------------------|----------------------------|
| 3420 | GROMACS | Task | New | Normal | Unify force and shellfc elements for modular simulator | Pascal Merz | 03/10/2020 09:50 PM | 2021-infrastructure-stable |
| 3419 | GROMACS | Task | New | Normal | Reduce / remove use of legacy t_state objects throughout modular simulator | Pascal Merz | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3418 | GROMACS | Task | New | Normal | Infrastructure improvements for modular simulator | Pascal Merz | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3416 | GROMACS | Task | New | Normal | Port post-submit matrix to Gitlab CI | Joe Jordan | 03/16/2020 05:50 PM | 2021-refactoring |
| 3415 | GROMACS | Task | New | Normal | Port Pre-submit matrix to Gitlab CI | Szilárd Páll | 03/23/2020 10:09 AM | 2021-refactoring |
| 3392 | GROMACS | Task | New | Low | Unify box correction for modular simulator | Pascal Merz | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 3382 | GROMACS | Task | Accepted | Normal | Split up t_inputrec | | 02/17/2020 05:28 PM | |
| 3370 | GROMACS | Task | New | High | Further improvements to GPU Buffer Ops and Comms | | 03/04/2020 01:38 PM | |
| 3366 | GROMACS | Task | New | Normal | Enforce compability of MdModules | | 02/28/2020 11:20 AM | |
| 3365 | GROMACS | Task | New | Low | consider making GPU bonded work independent from nonbonded | | 03/01/2020 01:11 PM | |
| 3361 | GROMACS | Task | New | Normal | Gitlab source archive contains files from build directory | Paul Bauer | 02/25/2020 10:13 AM | 2020.2 |
| 3360 | GROMACS | Task | New | Normal | investigate the future of DD dynamic load balancing with GPU offload | | 01/29/2020 11:23 AM | |
| 3357 | GROMACS | Task | New | Normal | Make sure "colvars" interoperates stably and smoothly with gromacs | | 03/04/2020 11:25 AM | |
| 3356 | GROMACS | Task | New | Normal | Expose setting of random seed to API | | 01/29/2020 06:16 PM | 2021 |
| 3353 | GROMACS | Task | New | Normal | Document gmx densmap output | | 01/23/2020 12:52 PM | |
| 3348 | GROMACS | Task | New | Normal | GPU LINCS and SETTLE: unify virial reduction | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3346 | GROMACS | Task | New | Normal | GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE. | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3345 | GROMACS | Task | New | Normal | GPU update-constraints: Reconsider the naming of coordinates buffer in constraints. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3344 | GROMACS | Task | New | Normal | GPU update-constraints: Better virial reduction. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3343 | GROMACS | Task | New | Normal | GPU SETTLE: Use different ordering for matrices. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3342 | GROMACS | Task | New | Normal | GPU SETTLE: Read only one index per water molecule. | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3341 | GROMACS | Task | New | Normal | GPU LINCS: Use analytical solution for the matrix A inversion. | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3340 | GROMACS | Task | New | Normal | GPU LINCS: Move more data to local/shared memory | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3339 | GROMACS | Task | New | Normal | GPU LINCS: Warp-level synchronization for coupled constraints | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3338 | GROMACS | Task | New | Normal | GPU update-constraints: Do not save intermediate coordinates if there is no constraints | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3337 | GROMACS | Task | New | Normal | GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels. | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3331 | GROMACS | Task | New | Low | Run physical validation tests in Gitlab | Paul Bauer | 02/27/2020 11:09 PM | future |
| 3330 | GROMACS | Task | New | Normal | Compile list of codepaths for testing task assignment | | 01/22/2020 10:03 AM | 2021-refactoring |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
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| 3329 | GROMACS | Task | New | Normal | Extend energy comparison testing framework | | 01/22/2020 09:51 AM | 2021-refactoring |
| 3327 | GROMACS | Task | New | Normal | Refactor workload flags | | 01/22/2020 09:45 AM | 2021-refactoring |
| 3326 | GROMACS | Task | New | Normal | Allow changing task assignment | | 01/22/2020 09:44 AM | 2021-refactoring |
| 3325 | GROMACS | Task | New | Normal | Allow complete re-initialization of a simulation | | 01/29/2020 05:13 PM | 2021-refactoring |
| 3324 | GROMACS | Task | New | Normal | Rework CMake handling of GPU code | | 01/22/2020 09:52 AM | 2021-refactoring |
| 3323 | GROMACS | Task | In Progress | Normal | Rework the StatePropagatorDataGpu | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3322 | GROMACS | Task | Accepted | Normal | Add reallocate(...) function that does not care about the contents of the buffer | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3321 | GROMACS | Task | Accepted | Normal | Add D2D wrapper | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3320 | GROMACS | Task | In Progress | Normal | Remove duplicating D2H/H2D wrappers in NBNXM | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3319 | GROMACS | Task | In Progress | Normal | Use DeviceBuffer instead of native GPU types in NBNXM | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3317 | GROMACS | Task | Resolved | Normal | Improve testing of the GPU code | Artem Zhmurov | 10/06/2020 12:15 PM | 2021-refactoring |
| 3316 | GROMACS | Task | Accepted | Normal | Context and Stream manager | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3315 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceContext | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring |
| 3314 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceStream | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring |
| 3312 | GROMACS | Task | In Progress | Normal | Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers | Artem Zhmurov | 03/20/2020 09:54 AM | 2021-refactoring |
| 3308 | GROMACS | Task | New | Normal | GPU update-constraints: Cycle counting for GPU launches | | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3306 | GROMACS | Task | New | Normal | Document gmx dos tool more clearly | Christian Blau | 01/20/2020 02:31 PM | future |
| 3300 | GROMACS | Task | New | Normal | Abandon docs/OpenCLTODOList.txt? | | 01/15/2020 02:46 PM | |
| 3297 | GROMACS | Task | Resolved | Normal | Require gcc > 5 | | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 3290 | GROMACS | Task | Resolved | Normal | Require CMake >= 3.12 | | 04/14/2020 02:45 PM | 2021-refactoring |
| 3289 | GROMACS | Task | New | Normal | Distinguish identifying and non-identifying inputs to API operations. | Eric Irrgang | 01/10/2020 11:30 AM | |
| 3287 | GROMACS | Task | New | Normal | Deprecate make_ndx, use select instead | | 01/23/2020 01:16 PM | |
| 3279 | GROMACS | Task | New | Low | Provide more advice for building client software | | 03/02/2020 11:54 AM | |
| 3275 | GROMACS | Task | New | Normal | Document Gitlab CI instead of Jenkins and releng | Paul Bauer | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3272 | GROMACS | Task | New | Normal | Port complete CI testing to Gitlab | Paul Bauer | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 3271 | GROMACS | Task | Resolved | Normal | Adopt PEP-518 for Python package build system configuration. | | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3268 | GROMACS | Task | New | Normal | add more Intel driver recommendations | | 12/26/2019 04:39 PM | |
| 3267 | GROMACS | Task | New | Normal | Document tools | | 12/26/2019 03:20 PM | future |
| 3264 | GROMACS | Task | New | Normal | Break up MdrunMpiTests | Paul Bauer | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 3262 | GROMACS | Task | New | High | Trjconv - dimer protein-ligand | | 12/20/2019 09:26 PM | |
| 3260 | GROMACS | Task | New | Low | keep up to with mdspan reference implementation | Christian Blau | 12/20/2019 01:16 PM | 2021-infrastructure-stable |
| 3258 | GROMACS | Task | New | Normal | GPU update-constraints: Enable free energy perturbation | Artem Zhmurov | 01/23/2020 11:54 AM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3256 | GROMACS | Task | New | Normal | Remove -nsteps option from mdrun | | 12/19/2019 12:12 PM | |
| 3255 | GROMACS | Task | New | Normal | Move benchmarking options from mdrun to a dedicated tool | | 12/19/2019 01:21 PM | |
| 3254 | GROMACS | Task | New | Normal | Remove support for generation of virtual sites to replace aromatic rings in standard residues | | 12/19/2019 12:13 PM | |
| 3252 | GROMACS | Task | New | Normal | Remove support for 32 bit architectures | | 03/01/2020 02:05 PM | |
| 3236 | GROMACS | Task | New | Normal | GPU update-constraints: Pulling support | Artem Zhmurov | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 3235 | GROMACS | Task | New | Normal | Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation | Christian Blau | 12/12/2019 03:46 PM | 2021-infrastructure-stable |
| 3229 | GROMACS | Task | New | Normal | Move checkpointing to the beginning of the MD step | | 01/16/2020 04:31 PM | 2021-infrastructure-stable |

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