

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 694 | Support Platforms | Feature | Feedback wanted | Normal | Write instructions/policy for issue handling | Rossen Apostolov | 05/31/2017 05:41 PM | |
| 1252 | TNG trajectory library | Bug | Feedback wanted | Normal | residual ids and atomIDs | Magnus Lundborg | 06/12/2013 10:35 AM | version 1 |
| 1377 | GROMACS | Feature | Feedback wanted | Low | Replica exchange if replicas not in ascendent T | David van der Spoel | 06/23/2016 03:48 PM | |
| 1442 | GROMACS | Bug | Feedback wanted | Normal | Not consistent solvation free energies differences | Michael Shirts | 07/11/2016 08:13 PM | |
| 1551 | Support Platforms | Bug | Feedback wanted | Normal | git index.lock issue | | 05/31/2017 05:37 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 | |
| 1880 | GROMACS | Bug | Feedback wanted | Normal | PP-PME load balancing issue | Berk Hess | 10/03/2018 09:45 PM | future |
| 2147 | GROMACS | Bug | Feedback wanted | Normal | Parrinello-Rahman barostat not properly working | | 06/06/2017 07:53 AM | |
| 2168 | GROMACS | Task | Feedback wanted | Normal | Design for multiple comparisons against same test reference data | | 05/08/2017 02:45 PM | future |
| 2218 | GROMACS | Feature | Feedback wanted | Normal | A tiny feature: damping for umbrella pull | | 08/16/2017 07:20 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 |
| 2482 | GROMACS | Bug | Feedback wanted | Normal | Atoms/molecules in freezegrps move and system crashes | | 05/18/2018 07:13 PM | |
| 2513 | GROMACS | Bug | Feedback wanted | Normal | ref_t and temperature incorrect with coulomb-type = user | Yu Du | 05/31/2018 04:05 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 | |
| 2828 | GROMACS | Bug | Feedback wanted | Normal | Installation issue on Power 9 system with SIMD support | | 01/18/2019 11:54 AM | |
| 2896 | GROMACS | Feature | Feedback wanted | Normal | Python packaging | | 01/16/2020 07:11 PM | 2021-refactoring |
| 3021 | GROMACS | Feature | Feedback wanted | Normal | Completion of docs for GPU developments | | 03/02/2020 03:58 PM | 2020.2 |
| 3028 | GROMACS | Bug | Feedback wanted | Normal | install fail on Centos 6 | | 07/15/2019 12:32 PM | |
| 3032 | GROMACS | Feature | Feedback wanted | Normal | Clean up dev-manual structure | | 12/11/2019 11:27 AM | 2021-infrastructure-stable |

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|------|------------------------|---------|-----------------|----------|--|---------------------|---------------------|----------------------------|
| 3047 | GROMACS | Task | Feedback wanted | Normal | Set required versions for GROMACS 2021 | | 02/20/2020 11:42 AM | |
| 3055 | GROMACS | Bug | Feedback wanted | Normal | Error in gmx xpm2ps | | 08/22/2019 03:27 PM | |
| 3058 | GROMACS | Bug | Feedback wanted | Normal | Error when using a large PME grid on a GPU | | 09/04/2019 07:26 PM | |
| 3077 | GROMACS | Task | Feedback wanted | Normal | PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor | | 11/01/2019 06:56 PM | |
| 3134 | GROMACS | Feature | Feedback wanted | Normal | gmxapi Python exception names may need improvement | Eric Irrgang | 10/13/2019 01:50 PM | |
| 3174 | GROMACS | Task | Feedback wanted | Low | Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs" | Eric Irrgang | 10/23/2019 06:34 PM | |
| 3243 | GROMACS | Bug | Feedback wanted | Normal | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning | | 12/27/2019 10:31 AM | |
| 3395 | GROMACS | Feature | Feedback wanted | Normal | Consider scripted composition of Dockerfiles | | 03/16/2020 12:16 PM | |
| 3413 | GROMACS | Bug | Feedback wanted | Normal | COMM Removal Failure in GROMACS 2020.1 | | 03/12/2020 02:31 PM | |
| 837 | Support Platforms | Task | Resolved | Low | Consider subproject organization of the Gromacs project | | 07/14/2014 12:07 PM | |
| 1229 | TNG trajectory library | Feature | Resolved | Normal | Selection groups | Magnus Lundborg | 11/29/2013 04:38 PM | version 1 |
| 1967 | Support Platforms | Bug | Resolved | Normal | Documentation pages generated by Jenkins do not render properly | | 08/27/2016 02:04 AM | |
| 2188 | TNG trajectory library | Feature | Resolved | High | Masses missing from TNG specification | Magnus Lundborg | 06/13/2017 05:08 PM | |
| 2254 | GROMACS | Feature | Resolved | Normal | GPU extensions for Google Tests | | 10/06/2020 12:15 PM | |
| 2451 | GROMACS | Feature | Resolved | Normal | Linear virtual sites with fixed distance | David van der Spoel | 09/16/2019 01:15 PM | |
| 2453 | GROMACS | Task | Resolved | High | PME OpenCL porting effort | Aleksei lupinov | 12/20/2019 12:18 PM | 2021 |
| 2522 | GROMACS | Task | Resolved | Normal | OpenCL context duplication | | 03/11/2020 04:15 PM | future |
| 2585 | GROMACS | Feature | Resolved | Normal | Infrastructure supporting external API | | 12/11/2019 12:39 PM | |
| 2628 | GROMACS | Bug | Resolved | Normal | GMXRC removes trailing colon from existing MANPATH | | 11/02/2020 11:45 AM | |
| 2859 | GROMACS | Task | Resolved | Normal | Change ArrayRef iterator type from pointer to std::iterator | | 06/26/2020 06:15 PM | |
| 2998 | GROMACS | Task | Resolved | Normal | Update Python detection | | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 3041 | GROMACS | Task | Resolved | Normal | Remove workaround for gcc bug 58265 | | 06/19/2020 04:45 PM | |
| 3125 | GROMACS | Bug | Resolved | Normal | OpenCL on Volta and Turing borken | | 02/27/2020 11:01 AM | 2020.2 |
| 3154 | GROMACS | Task | Resolved | Low | Update use of Python subprocess for >=3.5 | | 04/09/2020 10:15 PM | |
| 3219 | GROMACS | Bug | Resolved | Normal | MANPATH setting is fragile | | 11/02/2020 11:45 AM | |

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| 3271 | GROMACS | Task | Resolved | Normal | Adopt PEP-518 for Python package build system configuration. | | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3283 | GROMACS | Feature | Resolved | Normal | Support for the string method with swarms of trajectories in GROMACS | | 03/01/2020 01:16 PM | 2021 |
| 3285 | GROMACS | Feature | Resolved | Normal | Run simulations from the same tpr file with different random seeds | | 02/27/2020 11:22 PM | future |
| 3290 | GROMACS | Task | Resolved | Normal | Require CMake >= 3.12 | | 04/14/2020 02:45 PM | 2021-refactoring |
| 3297 | GROMACS | Task | Resolved | Normal | Require gcc > 5 | | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 3314 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceStream | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring |
| 3315 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceContext | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring |
| 3317 | GROMACS | Task | Resolved | Normal | Improve testing of the GPU code | Artem Zhmurov | 10/06/2020 12:15 PM | 2021-refactoring |
| 3380 | GROMACS | Bug | Resolved | Low | IBM VSX checks fail with gcc-10 | Erik Lindahl | 04/30/2020 01:30 PM | 2020.2 |
| 3393 | GROMACS | Feature | Resolved | Normal | Allow gmxapi.commandline_operation to use STDIN | Eric Irrgang | 02/25/2020 05:15 PM | 2021-infrastructure-stable |
| 3403 | GROMACS | Bug | Resolved | Normal | solvation free energy with couple-intramol set to no | | 12/10/2020 02:45 PM | |
| 3422 | GROMACS | Task | Resolved | Normal | Implement modular checkpointing for modular simulator | Pascal Merz | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 3441 | GROMACS | Bug | Resolved | Normal | Ewald surface-epsilon is incorrect | Berk Hess | 03/18/2020 11:15 PM | 2020.2 |
| 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 |
| 652 | GROMACS | Task | Blocked, need info | Normal | Change selection method implementation to use C++ | | 04/23/2017 08:05 PM | future |
| 921 | GROMACS | Feature | Blocked, need info | Normal | Default index groups and selections | | 07/11/2016 08:27 PM | |
| 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 | |
| 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 | |
| 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 | |
| 3101 | GROMACS | Bug | Blocked, need info | Normal | detect compilation failed | Erik Lindahl | 12/27/2019 10:52 AM | |
| 3265 | GROMACS | Bug | Blocked, need info | Low | regressiontests/complex fails on ppc64le | Erik Lindahl | 01/09/2020 05:00 PM | |
| 3310 | GROMACS | Bug | Blocked, need info | Low | Thread affinity on Mac OS | | 02/27/2020 11:10 PM | |
| 1030 | GROMACS | Feature | Fix uploaded | Low | adding -tu option to some analysis tools | Rossen Apostolov | 07/11/2016 08:22 PM | |
| 1985 | GROMACS | Bug | Fix uploaded | Low | CUDA build system refactoring awaiting review | | 12/20/2019 12:07 PM | 2021 |
| 2180 | Support Platforms | Feature | Fix uploaded | Low | relog matrices would work better with a hint for execution | | 05/19/2017 01:02 AM | |
| 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 |

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| 3408 | GROMACS | Bug | Fix uploaded | Normal | Gmxapi* tests segfault in rpmbuild | Eric Irrgang | 03/23/2020 01:27 PM | 2020.2 |
| 438 | GROMACS | Feature | In Progress | Low | New tool: g_correl | Alexey Shvetsov | 06/20/2014 10:38 AM | future |
| 629 | Support Platforms | Task | In Progress | Normal | List of users needs cleanup | Rossen Apostolov | 02/21/2018 02:07 PM | |
| 867 | GROMACS | Task | In Progress | Normal | Update Doxygen documentation for C++ code | Teemu Murtola | 07/11/2016 08:28 PM | |
| 868 | GROMACS | Feature | In Progress | Normal | Implement parallelization support to analysis framework | Kevin Boyd | 12/20/2019 11:59 AM | 2021 |
| 869 | GROMACS | Task | In Progress | Normal | Make analysis data histogramming and multipoint data easier to use in parallel | Teemu Murtola | 07/11/2016 08:28 PM | |
| 895 | GROMACS | Feature | In Progress | Normal | g_rmsf previous frame as reference | | 04/29/2013 07:39 PM | future |
| 920 | GROMACS | Task | In Progress | Normal | Add test framework for trajectory analysis modules | Teemu Murtola | 07/11/2016 08:27 PM | |
| 1010 | GROMACS | Task | In Progress | Normal | Better support for multiple AnalysisData datasets | Teemu Murtola | 07/11/2016 08:23 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 |
| 1083 | GROMACS | Feature | In Progress | Normal | Improve collective error/warning/note handling in mdrun | | 07/11/2016 08:21 PM | |
| 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 |
| 1198 | TNG trajectory library | Feature | In Progress | Normal | Full documentation for the high-level API | Magnus Lundborg | 06/25/2013 10:05 PM | version 2 |
| 1332 | GROMACS | Feature | In Progress | Normal | Supporting multiple end states instead of just A and B | Michael Shirts | 06/05/2018 03:58 PM | |
| 1367 | TNG trajectory library | Feature | In Progress | Normal | Break tng_io.c into smaller files | Magnus Lundborg | 10/25/2013 10:49 AM | version 1 |
| 1618 | GROMACS | Bug | In Progress | Normal | g_protonate segfaults unconditionally | Erik Lindahl | 08/17/2015 02:10 PM | |
| 1627 | GROMACS | Feature | In Progress | Normal | DPD integrator | | 07/11/2016 08:08 PM | |
| 1731 | Support Platforms | Bug | In Progress | Normal | document jenkins configuration and set up means to track changes | | 05/31/2017 06:13 PM | |
| 1815 | Support Platforms | Task | In Progress | Normal | implement and execute plan for new releng machinery | | 10/15/2016 05:37 PM | |
| 1843 | GROMACS | Bug | In Progress | Normal | pbcs=xy with 2 walls floating point exception with the verlet scheme | Berk Hess | 10/31/2016 11:35 AM | |
| 1879 | GROMACS | Task | In Progress | Low | make the GROMACS OpenCL kernel work on Gallium | | 11/30/2018 05:46 PM | future |
| 1925 | GROMACS | Task | In Progress | Normal | remove concept of unilateral global communication | | 12/29/2019 10:35 AM | 2021 |
| 2017 | GROMACS | Task | In Progress | Normal | Modularize simulation option storage and reading from mdp files | Christian Blau | 04/06/2018 06:07 PM | future |
| 2059 | GROMACS | Task | In Progress | Normal | Separate different types of data in t_state | | 12/27/2019 04:42 PM | 2021 |
| 2070 | GROMACS | Feature | In Progress | Normal | Physical validation testing | Michael Shirts | 01/03/2020 09:36 PM | future |
| 2071 | GROMACS | Task | In Progress | High | Low accuracy default settings yield incorrect liquid densities | Berk Hess | 01/05/2018 03:32 PM | |
| 2111 | GROMACS | Feature | In Progress | Normal | Implement Gaussian screening of electrostatics | | 02/23/2019 12:33 PM | |
| 2238 | GROMACS | Task | In Progress | Normal | GPU emulation mode support for rolling pruning missing | Berk Hess | 12/21/2017 03:21 PM | |

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|------|---------|---------|-------------|----------|--|------------------|---------------------|----------------------------|
| 2368 | GROMACS | Task | In Progress | Normal | update implementation of gmx msd | Kevin Boyd | 11/03/2018 07:43 PM | future |
| 2395 | GROMACS | Task | In Progress | Normal | break up commrec | Mark Abraham | 12/15/2019 11:51 AM | 2021-infrastructure-stable |
| 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 |
| 2452 | GROMACS | Task | In Progress | Normal | Reduce data dependencies in mdrun algorithms | Berk Hess | 03/14/2018 08:47 PM | |
| 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 | |
| 2675 | GROMACS | Task | In Progress | Normal | bonded CUDA offload task | | 02/12/2020 05:54 PM | 2021 |
| 2696 | GROMACS | Task | In Progress | Normal | ensure PME queue is flushed | Szilárd Páll | 12/31/2018 11:21 AM | future |
| 2698 | GROMACS | Task | In Progress | Normal | gmxapi documentation integration | | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 2734 | GROMACS | Bug | In Progress | Normal | regressiontests/kernel core dumps on ppc64le | Paul Bauer | 06/15/2019 04:12 PM | future |
| 2756 | GROMACS | Task | In Progress | Normal | gmxapi integration testing | | 01/16/2020 05:12 PM | 2021-refactoring |
| 2766 | GROMACS | Task | In Progress | Normal | Improve hardware option selection | Kevin Boyd | 12/20/2019 02:34 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 |
| 2818 | GROMACS | Task | In Progress | Normal | bonded GPU kernel fusion | Magnus Lundborg | 07/03/2019 09:01 PM | |
| 2834 | GROMACS | Task | In Progress | Normal | C++ matrix classes | Christian Blau | 12/29/2019 10:32 AM | 2021 |
| 2850 | GROMACS | Task | In Progress | Normal | assess Raptor Talos for testing | Szilárd Páll | 02/12/2019 01:14 PM | |
| 2890 | GROMACS | Feature | In Progress | Normal | GPU Halo Exchange | | 02/14/2020 12:41 PM | 2021 |
| 2891 | GROMACS | Feature | In Progress | Normal | PME/PP GPU communications | | 02/14/2020 12:40 PM | |
| 2915 | GROMACS | Feature | In Progress | High | GPU direct communications | | 02/14/2020 12:48 PM | |
| 2965 | GROMACS | Task | In Progress | Normal | Performance of GPU direct communications | | 02/14/2020 12:38 PM | 2021 |
| 2988 | GROMACS | Task | In Progress | Low | clean up and refactor code to modern standards | | 12/27/2019 04:37 PM | future |
| 2996 | GROMACS | Feature | In Progress | Normal | gmxapi execution model | Eric Irrgang | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 3010 | GROMACS | Task | In Progress | Normal | upgrade OpenCL stack on bs-gpu01 | | 12/20/2019 08:25 AM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task | In Progress | Normal | gmxapi example Python scripts | | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 3033 | GROMACS | Task | In Progress | Normal | Clean up and modernize googletest bundling and usage | | 01/16/2020 04:50 PM | 2021-refactoring |
| 3093 | GROMACS | Task | In Progress | High | rework GPU direct halo-exchange related force reduction complexities | | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3133 | GROMACS | Task | In Progress | Normal | Cookiecutter for sample_restraint | Eric Irrgang | 12/10/2019 01:59 PM | 2021-infrastructure-stable |
| 3186 | GROMACS | Task | In Progress | Normal | Update Constant/Variable naming in the PME GPU kernels. | | 10/30/2019 11:23 AM | |
| 3189 | GROMACS | Task | In Progress | High | implement heuristics for switching between different spread/gather kernel layouts | Jonathan Vincent | 01/29/2020 04:18 PM | 2021-infrastructure-stable |
| 3201 | GROMACS | Task | In Progress | Normal | Convert mdp parameters to key value tree | | 11/06/2019 06:06 PM | |

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|------|---------|---------|-------------|----------|---|-----------------|---------------------|------------------|
| 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 |
| 3249 | GROMACS | Bug | In Progress | Low | cmake bad tests for avx512 on AMD | Erik Lindahl | 02/26/2020 05:00 PM | |
| 3311 | GROMACS | Feature | In Progress | Normal | GPU infrastructure development | | 03/20/2020 09:54 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 |
| 3318 | GROMACS | Feature | In Progress | Normal | Use wrappers for the GPU buffer copy/allocations | Artem Zhmurov | 01/23/2020 12:01 PM | 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 |
| 3320 | GROMACS | Task | In Progress | Normal | Remove duplicating D2H/H2D wrappers in NBNXM | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3323 | GROMACS | Task | In Progress | Normal | Rework the StatePropagatorDataGpu | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 720 | GROMACS | Feature | Accepted | Low | permit pdb2gmx to choose a kind of HIS based on proton position | | 11/17/2016 03:51 PM | future |
| 907 | GROMACS | Feature | Accepted | Normal | Add tests for verifying installed headers | | 03/11/2014 09:15 PM | future |
| 1056 | GROMACS | Task | Accepted | Normal | status of fft5d_threads and fftw3_threads functionality | Mark Abraham | 07/11/2016 08:21 PM | |
| 1165 | GROMACS | Feature | Accepted | Low | Multi-SIMD binaries | | 12/20/2019 12:00 PM | future |
| 1192 | GROMACS | Feature | Accepted | Normal | Add support for Verlet scheme with Buckingham | Berk Hess | 07/11/2016 08:19 PM | |
| 1221 | GROMACS | Feature | Accepted | Normal | More generic position mapping for selections | | 06/10/2014 02:58 PM | future |
| 1328 | GROMACS | Feature | Accepted | Normal | Names for selection positions | | 07/11/2016 08:15 PM | |
| 1511 | GROMACS | Feature | Accepted | Normal | add PDBx (ie mmCIF) support | | 10/05/2018 07:14 PM | |
| 1781 | GROMACS | Task | Accepted | Normal | re-design benchmarking functionality | Mark Abraham | 12/20/2019 12:03 PM | future |
| 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 |
| 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 | |
| 1907 | GROMACS | Task | Accepted | Low | keeping compile- and run-time CPU/arch detection consistent | | 08/01/2016 10:09 PM | |
| 1919 | GROMACS | Bug | Accepted | Normal | static linking issues cause by hwloc support | | 10/12/2018 10:49 PM | future |
| 1943 | GROMACS | Task | Accepted | Low | make sure releases are submitted early for Debian Experimental | Szilárd Páll | 12/20/2019 12:05 PM | 2021 |
| 1964 | GROMACS | Feature | Accepted | Normal | "pull=no" should not produce warnings about "unknown" pull keywords | | 05/20/2016 02:37 PM | |
| 2054 | GROMACS | Feature | Accepted | High | PME on GPU | Aleksei lupinov | 12/20/2019 12:18 PM | future |
| 2166 | GROMACS | Task | Accepted | Normal | gmx trjconv functionality should check for mismatch between the tpr and the trajectory | | 05/05/2017 04:32 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 |
| 2194 | GROMACS | Feature | Accepted | Low | xvg output requested as an output option in place of xpm files | | 05/31/2017 04:26 PM | |
| 2233 | GROMACS | Bug | Accepted | Normal | replica exchange and -append bugged? | | 03/05/2018 01:38 PM | |

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| 2240 | GROMACS | Task | Accepted | Low | GPU emulation mode support for PME missing | | 09/16/2017 10:02 PM | |
| 2288 | GROMACS | Feature | Accepted | Low | gmx msd doesn't optimally handle missing input trajectory frames | | 11/10/2017 11:03 AM | |
| 2310 | GROMACS | Feature | Accepted | Low | Let mdrun dump coordinates with non-finite energy | | 10/03/2018 09:47 PM | future |
| 2448 | GROMACS | Task | Accepted | Normal | should mdrun -multidir permit only one directory? | | 03/21/2018 12:10 PM | |
| 2495 | GROMACS | Task | Accepted | Normal | replace -noconfout with mdp option | Mark Abraham | 12/28/2019 10:39 AM | 2021 |
| 2581 | GROMACS | Feature | Accepted | Normal | User interface for hybrid Monte Carlo | | 12/20/2019 12:24 PM | future |
| 2674 | GROMACS | Task | Accepted | Normal | Improve domain decomposition for bilayer systems | | 12/07/2018 04:03 PM | future |
| 2702 | GROMACS | Bug | Accepted | Normal | PME gather reduction race in OpenCL (and CUDA) | | 03/28/2019 03:14 PM | |
| 2706 | GROMACS | Task | Accepted | Normal | Rework classic QM/MM interface | | 12/02/2019 01:45 PM | 2021-infrastructure-stable |
| 2822 | GROMACS | Task | Accepted | Normal | Make nbnxn a module | Berk Hess | 12/18/2019 10:49 AM | future |
| 2875 | GROMACS | Task | Accepted | Normal | SIMD version of the free-energy kernel | Berk Hess | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2947 | GROMACS | Task | Accepted | Normal | make an end to end test for membed | | 09/24/2019 03:22 PM | future |
| 3071 | GROMACS | Bug | Accepted | Normal | complex.nbnxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions | Szilárd Páll | 02/25/2020 03:39 PM | 2020.2 |
| 3155 | GROMACS | Task | Accepted | Normal | Unify DD and CPU-GPU gather & scatter | Artem Zhmurov | 10/17/2019 03:50 PM | 2021-infrastructure-stable |
| 3183 | GROMACS | Task | Accepted | Normal | enable bonded interactions on GPU | | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 3203 | GROMACS | Task | Accepted | Normal | Tools should check that input is valid when first using it | Paul Bauer | 12/03/2019 05:26 PM | 2021-infrastructure-stable |
| 3234 | GROMACS | Bug | Accepted | Normal | Signal: Floating point exception Signal code: Floating point divide-by-zero | Erik Lindahl | 12/16/2019 03:40 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 |
| 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 |
| 3316 | GROMACS | Task | Accepted | Normal | Context and Stream manager | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3321 | GROMACS | Task | Accepted | Normal | Add D2D wrapper | 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 |
| 3355 | GROMACS | Feature | Accepted | Normal | New PME parallel (GPU) scheme | Jonathan Vincent | 02/12/2020 11:58 AM | |
| 3382 | GROMACS | Task | Accepted | Normal | Split up t_inputrec | | 02/17/2020 05:28 PM | |
| 3405 | GROMACS | Bug | Accepted | Normal | intermittent OpenCL regressiontest failures | | 03/02/2020 11:01 AM | |
| 3442 | GROMACS | Bug | Accepted | Normal | continuing mdrun with -deffnm and pulling does not work | | 03/15/2020 08:33 AM | |
| 665 | GROMACS | Task | New | Normal | Port existing trajectory analysis tools to use the new framework | | 07/14/2014 11:29 AM | future |
| 677 | GROMACS | Task | New | Normal | Make sure manual uses consistent style throughout | | 06/19/2014 11:49 AM | |
| 687 | Support Platforms | Feature | New | Normal | Add content on the front page | | 09/02/2019 01:08 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-------------------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 701 | GROMACS | Task | New | Normal | Add symbol visibility macros | | 03/02/2019 01:46 AM | future |
| 731 | GROMACS | Feature | New | Normal | pdb2gmx should warn about missing residues when bonds are too long | | 06/22/2014 10:55 AM | |
| 742 | GROMACS | Feature | New | Normal | Enhancing the performance of the free energy code | | 08/26/2019 04:55 PM | future |
| 760 | GROMACS | Feature | New | Low | Implement rigid body groups | Berk Hess | 12/30/2012 06:04 AM | future |
| 765 | GROMACS | Task | New | Normal | Improving serialization of data structures prior to communication | Mark Abraham | 05/13/2014 10:04 AM | future |
| 838 | GROMACS | Task | New | Normal | Improve generic error reporting routines | | 07/11/2016 08:29 PM | |
| 843 | GROMACS | Feature | New | Low | g_helixorient could benefit from more documentation | Erik Lindahl | 05/23/2014 02:02 PM | |
| 909 | GROMACS | Task | New | Normal | Reimplement displacement calculation module | | 07/14/2014 11:30 AM | future |
| 948 | GROMACS | Task | New | Normal | C++ thread synchronization primitives | Sander Pronk | 07/11/2016 08:24 PM | |
| 950 | GROMACS | Feature | New | Normal | Path/directory/filename handling in Gromacs | | 07/11/2016 08:24 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 |
| 986 | GROMACS | Task | New | Normal | Handling C++ out-of-memory errors | | 12/24/2014 08:42 PM | future |
| 987 | Support Platforms | Feature | New | Normal | Feature wishlist should be moved to Redmine | | 08/03/2012 12:22 PM | |
| 988 | GROMACS | Task | New | Normal | Definition of "public API" | | 08/28/2019 02:50 PM | future |
| 996 | GROMACS | Task | New | Normal | C++ MPI Framework | Roland Schulz | 07/14/2014 11:53 AM | future |
| 1017 | GROMACS | Task | New | Normal | C++ Vector/Matrix classes | | 07/11/2016 08:23 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 | |
| 1028 | GROMACS | Feature | New | Normal | Tool to calculate fraction of native contacts during simulation | | 11/01/2012 10:27 PM | |
| 1102 | GROMACS | Feature | New | Normal | Detect incompletely written itp files | | 06/19/2014 03:23 PM | |
| 1104 | GROMACS | Feature | New | Low | Implement dihedral restraints | | 02/06/2013 07:04 PM | future |
| 1105 | Benchmark suite | Feature | New | Normal | produce a benchmark suite | | 09/13/2016 10:31 PM | |
| 1106 | Benchmark suite | Feature | New | Normal | publish benchmark numbers | | 06/19/2014 12:08 PM | |
| 1120 | GROMACS | Feature | New | Low | Make build work with multi-configuration generators | | 06/03/2014 03:04 PM | future |
| 1137 | GROMACS | Feature | New | Normal | Proposal for integrator framework (do_md) in future GROMACS | Michael Shirts | 02/21/2017 12:48 AM | future |
| 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 | |
| 1140 | GROMACS | Task | New | Normal | Class design for passing options and data | | 07/11/2016 08:19 PM | |
| 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 |
| 1162 | GROMACS | Feature | New | Normal | Implement gb_saltconc | Berk Hess | 02/26/2013 05:33 PM | future |
| 1166 | GROMACS | Bug | New | Low | g_order is incorrect for unsaturated carbons | David van der Spoel | 02/06/2020 02:32 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 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 |
| 1170 | GROMACS | Task | New | Normal | mdlib reorganization | | 11/17/2016 03:47 PM | future |
| 1182 | GROMACS | Feature | New | Normal | improve trajectory writing to support parallel I/O | | 05/13/2014 10:42 AM | future |
| 1190 | GROMACS | Bug | New | Normal | Use of FORCE in setting cached variables | Mark Abraham | 06/17/2014 06:09 AM | |
| 1197 | TNG trajectory library | Feature | New | Normal | Rework the molecule descriptions | | 03/18/2013 04:16 PM | version 2 |
| 1199 | TNG trajectory library | Feature | New | Normal | residue numbering | Magnus Lundborg | 04/24/2013 09:33 AM | version 2 |
| 1200 | TNG trajectory library | Feature | New | Normal | Field for the PDB format 'segment identifier' | Magnus Lundborg | 04/24/2013 09:32 AM | version 2 |
| 1202 | TNG trajectory library | Feature | New | Normal | Other hash types | | 06/25/2013 10:02 PM | version 2 |
| 1206 | TNG trajectory library | Feature | New | Low | XTC Compression | | 10/25/2013 03:43 PM | version 2 |
| 1211 | GROMACS | Task | New | Low | improve use of preprocessor macros in CUDA kernels | Szilárd Páll | 01/12/2015 06:42 PM | future |
| 1214 | GROMACS | Task | New | Normal | Keep track of important changes for Changelog | Mark Abraham | 06/26/2013 11:24 AM | |
| 1235 | GROMACS | Bug | New | Normal | peptide dihedral angle definitions violate IUPAC | David van der Spoel | 06/19/2015 12:24 AM | future |
| 1246 | GROMACS | Task | New | Normal | expanded ensemble .tpr cannot be rerun | Michael Shirts | 06/19/2015 01:56 PM | |
| 1247 | GROMACS | Feature | New | Normal | fix hardcoded references to atom names in analysis tools | Mark Abraham | 06/12/2014 01:20 AM | future |
| 1303 | GROMACS | Feature | New | Normal | Adding lambda dependent distance for pull code | Michael Shirts | 07/11/2016 08:18 PM | |
| 1309 | Support Platforms | Task | New | Normal | Jenkins verification improvements | | 06/01/2017 02:34 PM | |
| 1323 | GROMACS | Task | New | Normal | determine future of existing tools for | David van der Spoel | 12/04/2018 11:53 AM | |
| 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 |
| 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 |
| 1347 | GROMACS | Feature | New | Normal | future of tables | Berk Hess | 01/09/2020 02:37 PM | future |
| 1354 | GROMACS | Bug | New | Normal | Constant acceleration NEMD is broken. | David van der Spoel | 01/09/2019 04:42 PM | |
| 1373 | GROMACS | Task | New | Low | Add missing nbxn tests | Mark Abraham | 06/09/2014 08:36 PM | |
| 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 |
| 1411 | GROMACS | Task | New | Normal | Future of thread_mpi | Mark Abraham | 02/26/2018 04:56 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 | |
| 1437 | GROMACS | Feature | New | Normal | Online help formatting improvements | | 06/04/2015 09:20 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 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 | |
| 1456 | GROMACS | Task | New | Low | remove the use of nbat->alloc/free pointers | Szilárd Páll | 06/20/2015 11:53 PM | |
| 1464 | GROMACS | Feature | New | Normal | implement PP-PME re-balancing | Szilárd Páll | 10/16/2015 08:34 AM | future |
| 1476 | GROMACS | Bug | New | Low | Odd behavior with verlet-buffer-drift | | 05/25/2016 01:45 AM | future |
| 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 | |
| 1489 | GROMACS | Feature | New | Normal | Don't solely rely on filename extension | | 04/30/2014 05:23 AM | |
| 1490 | GROMACS | Task | New | Normal | Usage of forward declarations vs typedef vs #include | Mark Abraham | 01/21/2015 10:23 AM | |
| 1498 | GROMACS | Feature | New | Low | g_dipoles does not work properly with ionic systems | David van der Spoel | 07/11/2016 08:11 PM | |
| 1500 | GROMACS | Feature | New | Normal | Post-5.0 feature clean-up plan | Mark Abraham | 08/26/2019 03:47 PM | |
| 1505 | GROMACS | Task | New | Normal | improve handling of logging | Mark Abraham | 01/02/2019 06:06 PM | |
| 1508 | Support Platforms | Task | New | Normal | Update master Jenkins build configurations | | 06/28/2014 03:59 AM | |
| 1509 | GROMACS | Task | New | Low | Reduce the distance dependence of shifted potentials for free energies if possible | Michael Shirts | 07/11/2016 08:10 PM | |
| 1515 | GROMACS | Task | New | Normal | improve g_bar output | Szilárd Páll | 07/11/2016 08:10 PM | |
| 1518 | GROMACS | Feature | New | Low | Enable automatic build checking for newer versions | Mark Abraham | 06/04/2014 04:13 PM | future |
| 1523 | GROMACS | Task | New | Normal | add missing code-paths to CUDA emulation kernel | | 07/11/2016 08:09 PM | |
| 1530 | GROMACS | Task | New | Low | Offer binary downloads | | 06/29/2014 02:58 PM | |
| 1536 | TNG trajectory library | Bug | New | Normal | TNG uses incorrect format for size_t on 32bit | | 06/28/2014 03:56 AM | |
| 1562 | GROMACS | Feature | New | Normal | introducing a Monte Carlo framework (first application: MC barostat) | Michael Shirts | 07/11/2016 08:08 PM | |
| 1568 | GROMACS | Bug | New | Low | inconsistent/incorrect threading checks and reporting in mdrun | | 05/25/2016 02:01 AM | |
| 1583 | GROMACS | Bug | New | Normal | gmx msd with mol flag requires excessive memory | | 12/18/2017 03:34 PM | |
| 1587 | GROMACS | Task | New | Normal | improve the configurability of regression tests | | 12/20/2019 12:02 PM | 2021 |
| 1601 | Support Platforms | Feature | New | Normal | use Git for Jenkins Config | | 05/24/2015 10:59 AM | |
| 1602 | GROMACS | Feature | New | Low | gmx order S per slice along all 3 axes | | 09/22/2014 07:25 AM | |
| 1625 | GROMACS | Feature | New | Normal | Gromacs Python API | | 03/02/2019 01:44 AM | future |
| 1634 | GROMACS | Feature | New | Normal | Boxed Molecular Dynamics | | 11/04/2014 04:40 PM | |
| 1635 | GROMACS | Feature | New | Normal | Proper Unicode support | | 06/18/2015 08:34 PM | |
| 1641 | GROMACS | Feature | New | Normal | Add toolchain file for Cray systems | | 06/06/2015 11:24 PM | |
| 1652 | GROMACS | Feature | New | Normal | Decide how to represent multiple lambda states internally | Michael Shirts | 06/05/2018 03:58 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-------------------|---------|--------|----------|--|------------------------|---------------------|----------------|
| 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 | |
| 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 | |
| 1655 | GROMACS | Bug | New | Normal | g_membed and box type | | 12/09/2014 01:33 PM | |
| 1658 | GROMACS | Feature | New | Normal | Electrostatics treatment for multiple lambda sites | Berk Hess | 07/11/2016 08:05 PM | |
| 1665 | GROMACS | Feature | New | Normal | improve free energy non-bonded kernel performance | | 08/26/2019 03:47 PM | future |
| 1666 | GROMACS | Feature | New | Normal | new approach for Verlet-scheme kernel generation | Erik Lindahl | 10/08/2018 07:04 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 | |
| 1670 | GROMACS | Feature | New | Normal | create mdrun option checking mini-tool | | 06/23/2016 04:06 PM | |
| 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 | |
| 1715 | GROMACS | Feature | New | Low | improve cycle counting GPU sharing and multi-sim | | 08/03/2016 12:32 PM | future |
| 1729 | GROMACS | Task | New | Normal | Resolve whether and how to resolve "state" variables stored in .tpr | | 05/13/2015 10:48 AM | future |
| 1730 | GROMACS | Bug | New | Normal | gmx compare does not compare all fields of a .tpr | | 06/12/2015 09:33 PM | future |
| 1732 | Support Platforms | Bug | New | Normal | review and extend jenkins tests setups, coverage | | 05/03/2016 05:30 AM | |
| 1745 | GROMACS | Task | New | Normal | Moving to C++11 after Gromacs-5.1 | | 06/01/2016 03:01 PM | |
| 1758 | GROMACS | Task | New | Normal | Verlet scheme reorganization / modularization | Mark Abraham | 07/20/2015 06:33 PM | future |
| 1768 | GROMACS | Task | New | Normal | decide future of command-line options vs env vars | | 11/03/2016 05:51 PM | future |
| 1770 | GROMACS | Bug | New | Normal | segmentation fault with free energy changes and multiple GPU's | | 07/14/2015 03:24 AM | |
| 1785 | GROMACS | Task | New | Low | no pV term written to energy file when pressure coupling is anisotropic | | 07/26/2015 01:47 PM | future |
| 1786 | GROMACS | Task | New | Normal | Python style standards in developer docs | Peter Kasson | 12/26/2019 03:15 PM | |
| 1793 | GROMACS | Task | New | Normal | cleanup of integration loop | Mark Abraham | 10/31/2018 10:49 PM | future |
| 1811 | GROMACS | Bug | New | Normal | Extrae build issues | | 12/13/2017 03:43 AM | |
| 1826 | GROMACS | Task | New | Normal | investigate non-optimal results with CPU-GPU balancing on AMD | Szilárd Páll | 12/20/2019 12:04 PM | future |
| 1827 | GROMACS | Bug | New | Low | cmake multi-configuration generator support partly broken | | 12/11/2017 05:20 PM | future |
| 1828 | GROMACS | Task | New | Normal | Exception handling in mdrun | | 10/07/2015 11:36 AM | |
| 1829 | GROMACS | Task | New | Normal | Future of thread level parallelism | | 11/18/2016 05:29 PM | |
| 1836 | Support Platforms | Bug | New | Normal | Support a way to retrigger part of matrix job | | 07/22/2017 12:30 AM | |
| 1842 | GROMACS | Feature | New | Normal | Replace XML with JSON | | 01/18/2018 05:12 PM | |
| 1849 | GROMACS | Feature | New | Normal | expanded ensemble -- Adaptive Integration Method | Christopher Mirabzadeh | 07/11/2016 08:01 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|--|-----------------|---------------------|----------------|
| 1852 | GROMACS | Task | New | Normal | Remove group scheme | | 03/03/2020 09:03 PM | future |
| 1854 | GROMACS | Feature | New | Normal | Remove all cyclic dependencies | | 05/25/2017 08:34 AM | |
| 1855 | GROMACS | Task | New | Normal | Convert preprocessor use so that symbols are always defined | | 06/28/2016 02:17 PM | |
| 1862 | GROMACS | Task | New | Normal | Fully replace t_topology by gmx_mtop_t | | 02/13/2019 04:53 PM | |
| 1864 | GROMACS | Feature | New | Normal | write tng files with energies | Magnus Lundborg | 07/11/2016 08:00 PM | |
| 1867 | GROMACS | Feature | New | Normal | make coupling implementations reversible | | 12/02/2015 07:43 AM | |
| 1876 | GROMACS | Task | New | Normal | Reorganize vector input passed to core MD routines | | 06/01/2016 01:59 PM | future |
| 1885 | GROMACS | Feature | New | Normal | DPD Thermostat | | 01/26/2016 10:17 AM | |
| 1900 | GROMACS | Feature | New | Normal | Implement some new errors in grompp | | 06/22/2016 05:20 PM | |
| 1934 | GROMACS | Bug | New | Normal | QMMM with ORCA: memory leaks, buffer overflows and much more | | 07/10/2016 09:26 AM | |
| 1936 | GROMACS | Task | New | Normal | treat default-able mdp fields as strings | | 04/02/2016 10:32 PM | future |
| 1937 | GROMACS | Task | New | Low | stop supporting changing CUDA host compiler | Mark Abraham | 10/15/2018 05:19 PM | future |
| 1947 | GROMACS | Task | New | Normal | Consider fixing corner case in TinyXML2 | Mark Abraham | 04/19/2016 01:40 AM | |
| 1948 | GROMACS | Feature | New | Low | add warning when non-identical GPUs are used | | 06/12/2017 08:45 PM | |
| 1953 | GROMACS | Feature | New | Low | use more regular polymorphism for GPU code | | 05/06/2016 10:06 PM | future |
| 1963 | GROMACS | Task | New | Low | collect examples of systems where users tried to do something that performed badly | Mark Abraham | 08/09/2016 07:30 AM | |
| 1966 | GROMACS | Feature | New | Low | Hydrogen mass repartiniog | | 05/25/2016 06:04 PM | future |
| 1971 | GROMACS | Task | New | Normal | Removing buggy features vs. keeping workflows | | 01/19/2018 01:36 PM | future |
| 1972 | GROMACS | Feature | New | Normal | external potential modules for refinement against experimental data | | 08/22/2018 05:03 PM | future |
| 1973 | GROMACS | Task | New | Normal | OpenCL implementation wish list | | 05/27/2016 03:42 PM | |
| 1974 | GROMACS | Feature | New | Normal | Report atom numbers and types in the error message about missed parameters | | 05/30/2016 09:24 AM | |
| 1994 | GROMACS | Feature | New | Low | explore using JIT for CUDA | | 07/11/2016 10:20 PM | future |
| 2001 | GROMACS | Feature | New | Normal | add MPI info to the mdrun log header | | 07/06/2016 05:21 PM | |
| 2003 | GROMACS | Task | New | Normal | reconsider various simd flags | | 07/07/2016 11:23 PM | |
| 2005 | GROMACS | Feature | New | Normal | Full Correlation Analysis (FCA) as Trajectory Analysis Module | Christian Blau | 02/07/2018 02:19 PM | future |
| 2009 | GROMACS | Task | New | Normal | improve command-line reporting of useful things | | 07/26/2016 12:54 PM | |
| 2010 | GROMACS | Task | New | Normal | Use size_t instead of int for indexing | | 07/01/2018 07:57 AM | |
| 2015 | GROMACS | Feature | New | Normal | Auto recovery from dd communication error | | 07/28/2016 03:17 PM | |
| 2018 | GROMACS | Feature | New | Normal | Pulling along a line between given points | | 07/27/2016 09:59 AM | |
| 2020 | GROMACS | Bug | New | Normal | Possible issue with md-vv integrator | Mark Abraham | 03/11/2017 08:30 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-------------------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 2034 | GROMACS | Feature | New | Normal | Unit tests for bonded forces | David van der Spoel | 06/29/2019 10:22 AM | future |
| 2035 | GROMACS | Task | New | Normal | A common trajectory analysis data exchange format | | 03/15/2017 05:46 PM | future |
| 2039 | GROMACS | Bug | New | Normal | mdrun -pinstride defaults are too confusing | | 12/13/2017 04:14 AM | |
| 2045 | GROMACS | Task | New | Normal | API design and language bindings | Peter Kasson | 01/29/2020 03:59 PM | |
| 2048 | GROMACS | Task | New | Normal | C++11: CUDA dependency on general headers | | 09/07/2016 10:30 PM | |
| 2052 | GROMACS | Bug | New | Low | trjconv does not recognize periodic molecules | David van der Spoel | 01/12/2018 11:05 AM | |
| 2053 | GROMACS | Task | New | Normal | refine notation in GPU code | | 12/20/2019 01:04 PM | 2021 |
| 2055 | GROMACS | Task | New | Low | Wiki registration is broken | | 01/20/2017 11:31 AM | |
| 2056 | GROMACS | Feature | New | Low | rename "gmx select" | | 10/03/2016 08:24 PM | |
| 2060 | GROMACS | Feature | New | Normal | Convert enum to enum class | | 10/17/2016 05:27 PM | |
| 2065 | GROMACS | Bug | New | Normal | thread-MPI internal errors | | 11/08/2018 03:43 PM | |
| 2068 | GROMACS | Feature | New | Normal | Access to low level classes | | 03/02/2019 01:37 AM | future |
| 2069 | GROMACS | Task | New | Low | Simple thread-parallelism inside routines | | 11/09/2016 06:06 PM | |
| 2080 | GROMACS | Feature | New | Normal | add grompp warning for suitability for domain decomposition | | 11/23/2016 03:03 PM | |
| 2084 | GROMACS | Task | New | Low | MPI and stderr/log output | | 11/28/2016 06:37 PM | |
| 2089 | GROMACS | Task | New | Normal | Encourage code review | | 01/10/2017 12:03 AM | |
| 2090 | GROMACS | Feature | New | Normal | redirecting stdout or stderr for testing | Mark Abraham | 12/15/2016 03:15 AM | |
| 2092 | GROMACS | Task | New | Normal | Tests running on GPU, and hardware assignment | | 12/19/2017 05:27 PM | future |
| 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 | |
| 2096 | Support Platforms | Bug | New | Normal | Redmine internal error with special characters | | 05/31/2017 08:48 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 |
| 2099 | Support Platforms | Feature | New | High | sharing accounts/credentials | | 12/06/2017 08:11 PM | |
| 2101 | GROMACS | Feature | New | Low | warninp could print the offending line, as well as its number | | 01/20/2017 03:06 PM | |
| 2113 | GROMACS | Bug | New | Normal | Google tests and execution order | | 03/05/2018 02:05 PM | |
| 2115 | GROMACS | Task | New | Normal | trjconv does too many things, and combinations of them work poorly | | 10/02/2018 09:04 AM | |
| 2118 | GROMACS | Feature | New | Low | More verbose comments requested in header of gmx distance -oxyz | | 02/08/2017 05:46 AM | |
| 2126 | GROMACS | Feature | New | Normal | implement native CUDA support in CMake | | 10/29/2019 09:03 PM | |
| 2132 | GROMACS | Feature | New | Normal | Intermediate code for xvg handling | | 03/08/2017 05:12 PM | future |
| 2133 | GROMACS | Task | New | Low | gmx traj needs reform | | 03/07/2017 02:02 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-------------------|---------|--------|----------|---|----------------|---------------------|----------------|
| 2137 | GROMACS | Feature | New | Normal | Preliminary refactoring of constraints and update machinery. | Michael Shirts | 03/11/2017 08:32 AM | future |
| 2139 | GROMACS | Feature | New | Normal | More precise/explicit documentation conventions | | 01/07/2018 11:54 PM | |
| 2149 | Support Platforms | Bug | New | Normal | gerrit server excessive CPU usage | | 04/05/2017 07:25 PM | |
| 2158 | GROMACS | Task | New | Normal | consider adding post-submit test that runs PME with 2xNN kernels | | 04/19/2017 08:04 PM | |
| 2169 | GROMACS | Task | New | Normal | remove 'continuation' mdp option | | 12/29/2019 10:31 AM | 2021 |
| 2175 | GROMACS | Task | New | Normal | improve clang static analyzer docs further | | 01/04/2018 04:13 PM | future |
| 2178 | GROMACS | Task | New | Normal | Move checks for specific warnings to source repo | | 05/12/2017 03:57 PM | |
| 2182 | GROMACS | Task | New | Low | de-duplicate code in densorder and hydorder | | 05/16/2017 11:29 AM | |
| 2185 | GROMACS | Task | New | Normal | add docs on MPI + CUDA w/wo MPS | | 05/24/2017 05:17 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 |
| 2207 | GROMACS | Feature | New | Normal | solvent excluded volume of large molecule with periodic boundary condition | | 06/16/2017 10:37 AM | |
| 2208 | GROMACS | Bug | New | Normal | cuFFT linking | | 06/30/2017 01:58 PM | |
| 2211 | GROMACS | Bug | New | Low | gmx writes normal output to stderr | | 03/05/2018 02:00 PM | future |
| 2216 | GROMACS | Task | New | Normal | GROMACS SIMD acceleration: generation 3 | Erik Lindahl | 07/17/2017 06:57 PM | future |
| 2217 | GROMACS | Bug | New | Low | GPU emulation and separate PME ranks doesn't work properly | | 12/12/2017 11:50 AM | |
| 2220 | GROMACS | Feature | New | Normal | report relevant env var behaviour to console | | 07/31/2017 09:40 PM | |
| 2221 | GROMACS | Task | New | Normal | Avoid preprocessor for SIMD functions | | 02/21/2018 01:43 PM | |
| 2224 | GROMACS | Feature | New | Normal | Proposed feature: conditional stop | Vedran Miletic | 12/20/2019 12:11 PM | 2021 |
| 2226 | GROMACS | Feature | New | Normal | Harmonise commands for exit in make_ndx and distance | | 08/04/2017 12:24 PM | |
| 2229 | GROMACS | Feature | New | High | Full Object Oriented Modularization of GROMACS MDRUN Codebase | Mark Abraham | 08/22/2018 05:03 PM | future |
| 2231 | GROMACS | Bug | New | Normal | convert-tpz aborts when saving subset of the system | | 01/12/2018 03:52 PM | |
| 2232 | GROMACS | Bug | New | Normal | pdb2gmx can't form special bonds with terminal patched atoms | | 12/03/2017 01:35 PM | |
| 2239 | GROMACS | Feature | New | Normal | split libgromacs into base and full | | 01/07/2019 01:47 AM | |
| 2241 | GROMACS | Bug | New | Low | refdata can segfault when reading | | 09/07/2017 11:57 AM | |
| 2248 | GROMACS | Feature | New | Normal | Label all SIMD functions as pure/nodiscard | | 02/04/2019 04:49 AM | |
| 2252 | GROMACS | Bug | New | Low | Memory allocation failures with large page sizes during PME tuning | | 12/14/2017 04:27 AM | |
| 2255 | GROMACS | Bug | New | Normal | nstlist override stopped affecting the input parameter listing | | 12/17/2017 08:05 AM | |
| 2282 | GROMACS | Feature | New | Normal | Density map toolset | Christian Blau | 03/21/2019 06:08 PM | future |
| 2283 | GROMACS | Feature | New | Normal | Force distribution analysis | Bernd Doser | 10/27/2017 11:44 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|--------|----------|--|--------------|---------------------|----------------------------|
| 2289 | GROMACS | Feature | New | Normal | gmx spatial add ability to perform over multiple reference structures | | 11/08/2017 12:31 AM | |
| 2294 | GROMACS | Task | New | Normal | Require identical hardware on nodes on parallel runs | | 11/19/2017 08:54 PM | |
| 2304 | GROMACS | Task | New | Normal | Document and propose tracking mdrun heuristics | | 10/03/2018 09:39 PM | future |
| 2341 | GROMACS | Task | New | Low | assess the state of building and using GROMACS on Windows | | 07/29/2019 11:09 PM | future |
| 2351 | GROMACS | Task | New | Normal | Avoid the SIMD module depending on non-trivial parts of Gromacs | | 12/14/2017 02:47 AM | future |
| 2353 | GROMACS | Task | New | Normal | improve on relative tolerance for constructing tables | | 12/20/2019 12:12 PM | 2021 |
| 2354 | GROMACS | Feature | New | Normal | develop configuration file support for control of task layout | | 09/19/2018 03:01 PM | future |
| 2360 | GROMACS | Bug | New | Low | error at counter reset with PME-only rank | | 01/05/2018 12:43 PM | future |
| 2362 | TNG trajectory library | Bug | New | Normal | tng_*_of_particle_nr_get() functions return wrong result for structures with multiple molecule types | | 12/21/2017 11:51 AM | |
| 2367 | GROMACS | Task | New | Normal | construct pbc_simd less often | | 09/24/2018 11:02 PM | future |
| 2371 | GROMACS | Task | New | Normal | mtop searching needs reconsideration | | 01/04/2018 11:54 AM | future |
| 2373 | GROMACS | Bug | New | Low | gmx -nice can't work | | 01/04/2018 11:17 AM | |
| 2375 | GROMACS | Task | New | Normal | Clarify execution phases for MD simulation | | 04/30/2019 12:59 PM | |
| 2376 | GROMACS | Task | New | Normal | max_mpi_ranks has wrong name | | 02/10/2018 11:03 AM | |
| 2379 | GROMACS | Task | New | Normal | check leftover FIXMEs in r2018 | Szilárd Páll | 12/31/2018 11:16 AM | future |
| 2380 | GROMACS | Bug | New | Low | cycle counter issues with separate PME rank + GPUs | | 01/16/2018 10:21 PM | |
| 2382 | GROMACS | Task | New | Normal | Simplify Doxygen guidelines | | 01/13/2018 12:40 AM | |
| 2383 | GROMACS | Task | New | Normal | Add JSON interface to write and read files | Paul Bauer | 01/16/2018 02:01 PM | future |
| 2393 | GROMACS | Bug | New | Normal | incorrect error message with omitted command line flag before its argument | | 01/24/2018 11:24 PM | |
| 2396 | GROMACS | Task | New | Normal | Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation | Paul Bauer | 12/02/2019 01:24 PM | 2021-infrastructure-stable |
| 2402 | GROMACS | Task | New | Normal | PME kernels general performance improvements | | 03/26/2018 10:41 AM | future |
| 2412 | GROMACS | Task | New | Normal | attempt to do better FFTW planning | | 03/15/2018 05:01 PM | |
| 2422 | GROMACS | Task | New | Normal | write C kernel for tables in Verlet scheme | | 02/26/2018 01:38 PM | |
| 2423 | GROMACS | Task | New | Normal | modernize constraints code | Mark Abraham | 09/19/2018 03:01 PM | future |
| 2425 | GROMACS | Task | New | Normal | testing multisim with multiple ranks per simulation | Mark Abraham | 12/20/2019 12:13 PM | 2021 |
| 2427 | GROMACS | Bug | New | Normal | gmx select gives syntax error for selection involving evaluating simple arithmetic expression | | 02/27/2018 05:15 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 | |
| 2429 | GROMACS | Feature | New | Normal | Add option of periodic chain topology to pdb2gmx | | 03/10/2018 01:01 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|-----------------|---------------------|----------------------------|
| 2435 | GROMACS | Task | New | Normal | identify and note about/tune task offload in GPU-bound runs | | 03/02/2018 04:08 PM | |
| 2442 | GROMACS | Task | New | Normal | Port gmx saxs and gmx sans to c++ | Joe Jordan | 06/28/2018 10:06 PM | future |
| 2445 | GROMACS | Task | New | Normal | Decide if/how to check for incompatible user input to mdrun for bonds and vsites | | 03/13/2018 02:02 PM | |
| 2456 | GROMACS | Task | New | Normal | Add a pull module external potential tests | | 03/15/2018 03:02 PM | |
| 2460 | GROMACS | Bug | New | Normal | Allow inclusion of user libraries through CMake cache variables | | 03/28/2018 08:47 PM | |
| 2462 | GROMACS | Task | New | Normal | consider adding STL misuse tests | | 03/23/2018 01:23 AM | |
| 2463 | GROMACS | Task | New | Low | PME GPU decomposition | | 03/26/2018 10:42 AM | |
| 2464 | GROMACS | Task | New | Normal | GPU performance goals overview | | 03/26/2018 10:42 AM | |
| 2468 | GROMACS | Bug | New | Low | incorrect GPU timing reported with OpenCL and domain decomposition | | 12/17/2018 01:28 PM | future |
| 2469 | GROMACS | Task | New | Normal | implement GPU timer reduction for reporting | | 03/27/2018 05:08 PM | |
| 2473 | GROMACS | Bug | New | Normal | mdrun sometimes stalls due to large coordinates with no constraints | | 04/04/2018 10:15 PM | |
| 2475 | GROMACS | Task | New | Normal | make OpenCL 1st class-citizen in the build system | | 12/20/2019 12:14 PM | 2021 |
| 2478 | GROMACS | Task | New | Low | avoid use of getenv in static initialization | | 04/13/2018 11:57 AM | |
| 2480 | GROMACS | Bug | New | Normal | pdb2gmx does not protonate correctly for united-atom Gromos | Mark Abraham | 12/20/2019 12:17 PM | 2021 |
| 2481 | GROMACS | Task | New | Low | Update gmx report-methods to write more method information | | 12/02/2019 01:22 PM | 2021-infrastructure-stable |
| 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 |
| 2488 | GROMACS | Task | New | Normal | use MPI non-blocking collectives to overlap pull comm | | 04/25/2018 04:19 PM | |
| 2490 | GROMACS | Task | New | Normal | evaluate two-step communicators | Szilárd Páll | 10/03/2018 09:47 PM | future |
| 2491 | GROMACS | Feature | New | Low | Allow constant bias AWH simulations | Viveca Lindahl | 06/05/2018 10:38 PM | future |
| 2492 | GROMACS | Task | New | Normal | implement force calculation via ForceProviders containing collections of IForceProvider | Mark Abraham | 09/19/2018 03:13 PM | future |
| 2496 | GROMACS | Task | New | Low | find system xdr properly | | 05/02/2018 02:19 PM | |
| 2498 | GROMACS | Task | New | Normal | OpenCL memory pinning/mapping | | 12/20/2019 12:18 PM | future |
| 2501 | GROMACS | Task | New | Normal | Documentation section on log file contents | Kevin Boyd | 10/03/2018 09:48 PM | future |
| 2514 | GROMACS | Task | New | Normal | PME OpenCL reductions with intrinsics | | 05/31/2018 12:27 AM | future |
| 2516 | GROMACS | Task | New | Low | Support PME OpenCL execution width < 16 | Aleksei lupinov | 06/05/2019 05:32 PM | |
| 2518 | GROMACS | Task | New | Normal | redesign task-assignment code for OpenCL | | 12/20/2019 12:19 PM | future |
| 2519 | GROMACS | Task | New | High | Improve/remove PME OpenCL kernel barriers | | 02/15/2019 06:34 PM | |
| 2520 | GROMACS | Task | New | Normal | Treat OpenCL kernel width more diligently | | 05/24/2018 06:21 PM | |
| 2521 | GROMACS | Task | New | Normal | Implement alternating PME/NB wait for OpenCL | | 10/15/2018 12:39 PM | |
| 2524 | GROMACS | Task | New | Normal | struct alignment/packing for OpenCL host & device code | | 12/20/2019 12:20 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 2526 | GROMACS | Bug | New | Normal | Bug of gmx hbond | | 05/30/2018 03:12 PM | |
| 2527 | GROMACS | Task | New | Normal | Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL) | | 10/30/2018 04:06 AM | future |
| 2528 | GROMACS | Task | New | Normal | PME GPU tuning | | 12/31/2018 11:18 AM | future |
| 2530 | GROMACS | Task | New | Normal | consider using CUDA Driver API | | 09/23/2018 11:47 PM | future |
| 2531 | GROMACS | Task | New | Low | Consider optimizing tabulated data access on GPU | | 07/30/2018 12:31 PM | |
| 2532 | GROMACS | Task | New | Normal | enable queue priorities in OpenCL | | 05/29/2018 02:29 PM | |
| 2535 | GROMACS | Task | New | Normal | consider compiling opencl fft kernels once | | 05/31/2018 01:33 PM | |
| 2537 | GROMACS | Task | New | Normal | Simplify PME solve reduction | Aleksei lupinov | 12/20/2019 12:21 PM | future |
| 2538 | GROMACS | Task | New | Normal | organize more of the PME GPU code along task-specific lines | Mark Abraham | 05/31/2018 05:41 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 |
| 2545 | GROMACS | Feature | New | Normal | Should grompp fix periodicity of input files? | David van der Spoel | 10/03/2018 11:32 PM | future |
| 2546 | GROMACS | Task | New | Normal | Add more assertions to AWH code | Viveca Lindahl | 06/06/2018 11:20 AM | future |
| 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 |
| 2555 | GROMACS | Bug | New | Low | building GROMACS 2018.2 | | 07/03/2018 11:41 PM | |
| 2556 | GROMACS | Feature | New | Normal | make default selections suitable for DNA and RNA | Mark Abraham | 06/20/2018 01:48 PM | |
| 2563 | GROMACS | Bug | New | Normal | Windows 7 Compilation with GPU support | | 07/02/2018 09:58 AM | |
| 2564 | GROMACS | Bug | New | Normal | Result Summary Different For Jobs With Different Numbers of Nodes | | 07/05/2018 02:39 PM | |
| 2567 | GROMACS | Bug | New | Normal | make check fails at test 23 SIMD errors | | 07/10/2018 09:35 AM | |
| 2568 | GROMACS | Bug | New | Low | gmx editconf -rotate does not rotate the box | | 07/10/2018 10:27 AM | future |
| 2570 | GROMACS | Feature | New | Normal | Better string formatting and printing | | 05/02/2019 12:20 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 | |
| 2574 | GROMACS | Feature | New | Normal | iForceSchedule Abstraction | Prashanth Kanduri | 03/29/2019 05:20 PM | future |
| 2576 | GROMACS | Bug | New | Normal | gmx potential -correct outputs the wrong potential | | 07/25/2018 02:58 PM | |
| 2579 | GROMACS | Feature | New | Normal | Add dimensionality option to gmx trjconv -center | | 07/19/2018 04:53 PM | future |
| 2590 | GROMACS | Task | New | Normal | Essential Dynamics as module providing forces | Christian Blau | 08/22/2018 05:03 PM | future |
| 2594 | GROMACS | Feature | New | Normal | Multi-level GMX API | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2595 | GROMACS | Task | New | Normal | Reusable Utilities for Schedules | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2596 | GROMACS | Feature | New | Normal | Constant potential method | Benson Muite | 05/10/2019 09:54 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 2598 | GROMACS | Bug | New | Normal | Tools using read_next_x cannot read TNG files with sanitizers | | 10/15/2018 01:16 PM | future |
| 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 | |
| 2601 | GROMACS | Feature | New | Normal | Free energy calculations, soft-core potential | Vytautas Gapsys | 02/10/2020 11:29 AM | future |
| 2602 | GROMACS | Bug | New | Low | build information gets outdated if build tree is reused | | 08/13/2018 09:04 PM | |
| 2603 | GROMACS | Task | New | Normal | Add ability to properly check coordinate files during testing | Paul Bauer | 10/15/2018 01:16 PM | future |
| 2606 | GROMACS | Bug | New | Normal | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert | | 08/10/2018 01:48 AM | |
| 2607 | GROMACS | Bug | New | Normal | Grompp becomes extremely slow when many pull groups are present | | 08/11/2018 08:54 AM | |
| 2608 | GROMACS | Task | New | Normal | Remove code duplication between OpenCL and CUDA | | 09/24/2018 12:47 PM | |
| 2611 | GROMACS | Bug | New | Normal | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX | | 08/14/2018 07:03 PM | |
| 2616 | GROMACS | Task | New | Normal | Model for MD state | | 09/14/2018 05:12 PM | |
| 2621 | GROMACS | Task | New | Normal | Fine-Grained API to Describe Force Calculation and Neighbourhood Search | Prashanth Kanduri | 08/22/2018 11:36 AM | future |
| 2622 | GROMACS | Feature | New | Low | Reduce severity of Berendsen warning | | 08/23/2018 11:16 PM | future |
| 2624 | GROMACS | Bug | New | Normal | GPU build system not robust enough | | 09/05/2018 02:00 AM | |
| 2632 | GROMACS | Task | New | Low | make sure cmake defines proper hwloc versionc with cross-compilation enabled | | 12/03/2018 01:35 PM | future |
| 2637 | GROMACS | Bug | New | High | gmx solvate tears apart molecules | | 09/11/2018 07:43 PM | |
| 2643 | GROMACS | Feature | New | Low | mdp options and/or docs for anisotropic aspects of implementations | | 09/12/2018 02:23 PM | |
| 2644 | GROMACS | Task | New | Normal | Replace compute_globals | Mark Abraham | 09/24/2018 05:51 PM | future |
| 2645 | GROMACS | Bug | New | Normal | Security | | 09/28/2018 01:16 PM | |
| 2649 | GROMACS | Bug | New | Normal | Virial calculation necessary for correct energy calculation on GPU | | 12/17/2018 02:32 PM | future |
| 2650 | GROMACS | Task | New | Normal | revise OpenCL stack recommendations | | 12/31/2018 11:19 AM | future |
| 2657 | GROMACS | Bug | New | Normal | Biphasic tutorial | | 09/28/2018 10:02 AM | |
| 2658 | GROMACS | Task | New | Normal | Secondary structure assignment via DSSP as native gromacs code | Christian Blau | 10/09/2018 04:51 PM | future |
| 2660 | GROMACS | Task | New | Low | rework OpenCL nbxn kernel constants | Szilárd Páll | 12/28/2019 10:53 AM | future |
| 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 |
| 2670 | GROMACS | Task | New | Low | remove old/backward compatibility OpenCL support from releng | | 10/04/2018 06:06 PM | |
| 2671 | GROMACS | Task | New | Normal | replace constants like M_PI | | 12/20/2019 01:17 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|----------|---------------------|----------------|
| 2672 | GROMACS | Task | New | Normal | check & document execution width requirements in OpenCL | | 12/31/2018 11:20 AM | future |
| 2682 | GROMACS | Task | New | Normal | Add MSAN configuration | | 10/09/2018 06:28 PM | |
| 2686 | GROMACS | Task | New | Normal | add tests for gpu bonded interactions | | 12/27/2019 04:40 PM | 2021 |
| 2693 | GROMACS | Bug | New | Normal | Several memory leaks in mdrun | | 12/18/2018 04:22 AM | future |
| 2695 | GROMACS | Task | New | Low | bonded GPU module timing | | 12/27/2019 04:40 PM | 2021 |

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