

## Issues

| #    | Project           | Tracker | Status          | Priority | Subject   | Assignee | Updated             | Target version             |
|------|-------------------|---------|-----------------|----------|---|----------|---------------------|----------------------------|
| 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 |                            |
| 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 |                            |
| 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 |                            |
| 2637 | GROMACS           | Bug     | New             | High     | gmx solvate tears apart molecules   |          | 09/11/2018 07:43 PM |                            |
| 3210 | GROMACS           | Bug     | New             | High     | rerun does not reproduce dVcoul/dl  |          | 12/27/2019 10:45 AM |                            |
| 2935 | Support Platforms | Bug     | New             | High     | redmine issue updates about Gerrit uploads stopped working  |          | 06/11/2019 01:42 PM | current                    |
| 2915 | GROMACS           | Feature | In Progress     | High     | GPU direct communications   |          | 02/14/2020 12:48 PM |                            |
| 2099 | Support Platforms | Feature | New             | High     | sharing accounts/credentials  |          | 12/06/2017 08:11 PM |                            |
| 2519 | GROMACS           | Task    | New             | High     | Improve/remove PME OpenCL kernel barriers   |          | 02/15/2019 06:34 PM |                            |
| 2792 | GROMACS           | Task    | New             | High     | Improvement of PME gather and spread CUDA kernels   |          | 03/18/2020 03:57 PM |                            |
| 3082 | GROMACS           | Task    | New             | High     | move launch/synchronization points to clarify task dependencies   |          | 12/27/2019 04:21 PM | 2021                       |
| 3093 | GROMACS           | Task    | In Progress     | High     | rework GPU direct halo-exchange related force reduction complexities  |          | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3262 | GROMACS           | Task    | New             | High     | Trjconv - dimer protein-ligand  |          | 12/20/2019 09:26 PM |                            |
| 3370 | GROMACS           | Task    | New             | High     | Further improvements to GPU Buffer Ops and Comms  |          | 03/04/2020 01:38 PM |                            |
| 1583 | GROMACS           | Bug     | New             | Normal   | gmx msd with mol flag requires excessive memory   |          | 12/18/2017 03:34 PM |                            |
| 1655 | GROMACS           | Bug     | New             | Normal   | g_membed and box type   |          | 12/09/2014 01:33 PM |                            |
| 1730 | GROMACS           | Bug     | New             | Normal   | gmx compare does not compare all fields of a .tpr   |          | 06/12/2015 09:33 PM | future                     |
| 1770 | GROMACS           | Bug     | New             | Normal   | segmentation fault with free energy changes and multiple GPU's  |          | 07/14/2015 03:24 AM |                            |
| 1811 | GROMACS           | Bug     | New             | Normal   | Extrae build issues   |          | 12/13/2017 03:43 AM |                            |
| 1919 | GROMACS           | Bug     | Accepted        | Normal   | static linking issues cause by hwloc support  |          | 10/12/2018 10:49 PM | future                     |
| 1934 | GROMACS           | Bug     | New             | Normal   | QMMM with ORCA: memory leaks, buffer overflows and much more  |          | 07/10/2016 09:26 AM |                            |
| 2039 | GROMACS           | Bug     | New             | Normal   | mdrun -pinstride defaults are too confusing   |          | 12/13/2017 04:14 AM |                            |
| 2065 | GROMACS           | Bug     | New             | Normal   | thread-MPI internal errors  |          | 11/08/2018 03:43 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 |                            |
| 2113 | GROMACS           | Bug     | New             | Normal   | Google tests and execution order  |          | 03/05/2018 02:05 PM |                            |
| 2147 | GROMACS           | Bug     | Feedback wanted | Normal   | Parrinello-Rahman barostat not properly working   |          | 06/06/2017 07:53 AM |                            |
| 2208 | GROMACS           | Bug     | New             | Normal   | cuFFT linking   |          | 06/30/2017 01:58 PM |                            |

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|------|---------|---------|-----------------|----------|---|----------|---------------------|----------------|
| 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 |                |
| 2233 | GROMACS | Bug     | Accepted        | Normal   | replica exchange and -append bugged?  |          | 03/05/2018 01:38 PM |                |
| 2255 | GROMACS | Bug     | New             | Normal   | nstlist override stopped affecting the input parameter listing                                |          | 12/17/2017 08:05 AM |                |
| 2390 | GROMACS | Bug     | Feedback wanted | Normal   | GROMACS build system should check for valid nvcc flags before use                             |          | 12/20/2019 12:13 PM | 2021           |
| 2393 | GROMACS | Bug     | New             | Normal   | incorrect error message with omitted command line flag before its argument                    |          | 01/24/2018 11:24 PM |                |
| 2427 | GROMACS | Bug     | New             | Normal   | gmx select gives syntax error for selection involving evaluating simple arithmetic expression |          | 02/27/2018 05:15 PM |                |
| 2460 | GROMACS | Bug     | New             | Normal   | Allow inclusion of user libraries through CMake cache variables                               |          | 03/28/2018 08:47 PM |                |
| 2473 | GROMACS | Bug     | New             | Normal   | mdrun sometimes stalls due to large coordinates with no constraints                           |          | 04/04/2018 10:15 PM |                |
| 2482 | GROMACS | Bug     | Feedback wanted | Normal   | Atoms/molecules in freezegrps move and system crashes   |          | 05/18/2018 07:13 PM |                |
| 2526 | GROMACS | Bug     | New             | Normal   | Bug of gmx hbond  |          | 05/30/2018 03:12 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 |                |
| 2576 | GROMACS | Bug     | New             | Normal   | gmx potential -correct outputs the wrong potential  |          | 07/25/2018 02:58 PM |                |
| 2598 | GROMACS | Bug     | New             | Normal   | Tools using read_next_x cannot read TNG files with sanitizers                                 |          | 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 |                |
| 2611 | GROMACS | Bug     | New             | Normal   | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX                            |          | 08/14/2018 07:03 PM |                |
| 2624 | GROMACS | Bug     | New             | Normal   | GPU build system not robust enough  |          | 09/05/2018 02:00 AM |                |
| 2628 | GROMACS | Bug     | Resolved        | Normal   | GMXRC removes trailing colon from existing MANPATH  |          | 11/02/2020 11:45 AM |                |
| 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         |
| 2657 | GROMACS | Bug     | New             | Normal   | Biphasic tutorial   |          | 09/28/2018 10:02 AM |                |
| 2693 | GROMACS | Bug     | New             | Normal   | Several memory leaks in mdrun   |          | 12/18/2018 04:22 AM | future         |
| 2702 | GROMACS | Bug     | Accepted        | Normal   | PME gather reduction race in OpenCL (and CUDA)  |          | 03/28/2019 03:14 PM |                |
| 2707 | GROMACS | Bug     | New             | Normal   | Installed OpenCL files include clh file from gpu_utils directory                              |          | 10/30/2018 04:02 AM |                |

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|------|---------|---------|-----------------------|----------|---|----------|---------------------|----------------|
| 2762 | GROMACS | Bug     | Blocked,<br>need info | Normal   | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads              |          | 07/01/2019 11:26 PM |                |
| 2763 | GROMACS | Bug     | New                   | Normal   | GMXAPI layout / grouping in development docs "modules" page                       |          | 12/14/2018 12:49 PM | future         |
| 2785 | GROMACS | Bug     | New                   | Normal   | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG        |          | 11/30/2018 02:36 PM |                |
| 2788 | GROMACS | Bug     | New                   | Normal   | PME will not run on AMD GPU with NVidia GPU present                               |          | 01/03/2019 02:24 PM |                |
| 2828 | GROMACS | Bug     | Feedback<br>wanted    | Normal   | Installation issue on Power 9 system with SIMD support                            |          | 01/18/2019 11:54 AM |                |
| 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 |                |
| 2869 | GROMACS | Bug     | New                   | Normal   | GPU detection error only issued as a note to the log                              |          | 03/05/2019 04:09 PM |                |
| 2870 | GROMACS | Bug     | New                   | Normal   | GPU detection error message missing from the output                               |          | 03/05/2019 03:55 PM |                |
| 2872 | GROMACS | Bug     | New                   | Normal   | gmx solvate and genion topology update  |          | 02/27/2019 10:18 AM |                |
| 2873 | GROMACS | Bug     | New                   | Normal   | Simple way to get last frame from trajectory                                      |          | 02/28/2019 11:14 PM |                |
| 2883 | GROMACS | Bug     | New                   | Normal   | essentialdynamics fail with Intel MPI   |          | 03/08/2019 03:10 AM |                |
| 2897 | GROMACS | Bug     | New                   | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build                     |          | 04/04/2019 06:24 PM |                |
| 2902 | GROMACS | Bug     | New                   | Normal   | 2019.1 equilibration issue? (Intel 2018u3)  |          | 04/30/2019 08:17 AM |                |
| 2907 | GROMACS | Bug     | New                   | Normal   | Gromacs autocompletion appears to be broken with ZSH                              |          | 07/16/2019 04:46 AM |                |
| 2924 | GROMACS | Bug     | New                   | Normal   | Failing version check when reading new tpr file with older gromacs version        |          | 04/12/2019 10:52 AM |                |
| 2948 | GROMACS | Bug     | New                   | Normal   | SIMD support detected as none on AMD R5 2500U                                     |          | 05/21/2019 12:58 PM |                |
| 2949 | GROMACS | Bug     | New                   | Normal   | cmake fails when building mdrun only  |          | 07/08/2019 10:04 AM |                |
| 2954 | GROMACS | Bug     | New                   | Normal   | genion changes residue numbering  |          | 05/26/2019 12:08 AM |                |
| 2958 | GROMACS | Bug     | New                   | Normal   | Compiling master (to become 2020) using CUDA 9.0                                  |          | 03/02/2020 03:57 PM | 2020.2         |
| 2974 | GROMACS | Bug     | New                   | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                 |          | 02/25/2020 03:52 PM | 2020.2         |
| 2978 | GROMACS | Bug     | New                   | Normal   | Some suggestions about the gmx current tool                                       |          | 06/13/2019 12:41 PM |                |
| 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 |                |
| 2981 | GROMACS | Bug     | New                   | Normal   | segfault in opencl build  |          | 06/18/2019 03:30 AM |                |
| 2987 | GROMACS | Bug     | New                   | Normal   | assess the bonded GPU task assignment default                                     |          | 12/20/2019 01:06 PM | 2021           |
| 3000 | GROMACS | Bug     | New                   | Normal   | CMake "webpage" target does not fail when it should                               |          | 06/25/2019 02:43 PM |                |
| 3028 | GROMACS | Bug     | Feedback<br>wanted    | Normal   | install fail on Centos 6  |          | 07/15/2019 12:32 PM |                |
| 3042 | GROMACS | Bug     | New                   | Normal   | core dump error in grompp command   |          | 10/09/2019 07:30 PM |                |

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|------|---------|---------|-----------------|----------|---|----------|---------------------|----------------------------|
| 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 |                            |
| 3054 | GROMACS | Bug     | New             | Normal   | Missing dihedral define   |          | 08/02/2019 05:47 PM |                            |
| 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 |                            |
| 3068 | GROMACS | Bug     | New             | Normal   | Misleading warning on rerun   |          | 08/26/2019 03:44 PM |                            |
| 3073 | GROMACS | Bug     | New             | Normal   | Total potential energy goes crazy, but I don't know why this happens.   |          | 09/04/2019 07:25 PM |                            |
| 3083 | GROMACS | Bug     | New             | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build  |          | 09/10/2019 11:56 AM |                            |
| 3086 | GROMACS | Bug     | New             | Normal   | gmxapi fails with MPI build of GROMACS 2020   |          | 09/25/2019 04:18 PM |                            |
| 3088 | GROMACS | Bug     | New             | Normal   | Reference to theory needed for cylindrical pull geometry  |          | 09/13/2019 11:26 AM |                            |
| 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                       |
| 3125 | GROMACS | Bug     | Resolved        | Normal   | OpenCL on Volta and Turing broken   |          | 02/27/2020 11:01 AM | 2020.2                     |
| 3127 | GROMACS | Bug     | New             | Normal   | mddrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia   |          | 10/09/2019 05:33 PM |                            |
| 3165 | GROMACS | Bug     | New             | Normal   | task assignment silent abort  |          | 10/18/2019 07:46 PM |                            |
| 3166 | GROMACS | Bug     | New             | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1  |          | 10/19/2019 09:13 PM |                            |
| 3196 | GROMACS | Bug     | New             | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |          | 11/01/2019 11:28 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 |
| 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 |                            |
| 3209 | GROMACS | Bug     | New             | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting   |          | 11/19/2019 11:36 AM |                            |
| 3213 | GROMACS | Bug     | New             | Normal   | Having a local residuetypes.dat for custom force field  |          | 11/21/2019 09:18 PM |                            |
| 3214 | GROMACS | Bug     | New             | Normal   | Out-of-bounds, overflow and incorrect outputs in gmx spatial  |          | 11/25/2019 04:11 PM |                            |
| 3219 | GROMACS | Bug     | Resolved        | Normal   | MANPATH setting is fragile  |          | 11/02/2020 11:45 AM |                            |
| 3223 | GROMACS | Bug     | New             | Normal   | unit test failures give verify -1   |          | 12/02/2019 11:58 AM |                            |
| 3227 | GROMACS | Bug     | New             | Normal   | solvate does not check return status of gmx_file_rename   |          | 12/04/2019 01:43 PM |                            |
| 3233 | GROMACS | Bug     | New             | Normal   | clang-format incorrectly aligning altered function arguments  |          | 12/13/2019 12:41 PM |                            |
| 3239 | GROMACS | Bug     | New             | Normal   | GPU DD direct communication with GPU update error with RF   |          | 12/14/2019 05:15 PM |                            |

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|------|------------------------|---------|-----------------|----------|--|----------|---------------------|----------------------------|
| 3240 | GROMACS                | Bug     | New             | Normal   | segv with GPU DD direct communication with GPU update and -dlb off                       |          | 01/15/2020 06:16 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 |                            |
| 3273 | GROMACS                | Bug     | New             | Normal   | gmxapi setup.py complains too much   |          | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3274 | GROMACS                | Bug     | New             | Normal   | Remove ARM NEON SIMD   |          | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3281 | GROMACS                | Bug     | New             | Normal   | Test data directory GMX_RELEASE_ASSERT triggers  |          | 01/06/2020 08:07 PM |                            |
| 3301 | GROMACS                | Bug     | New             | Normal   | pdb2gmx adding hydrogen  |          | 01/15/2020 10:17 PM |                            |
| 3305 | GROMACS                | Bug     | New             | Normal   | Case gives FPE with Debug build when GPU update is enabled                               |          | 01/21/2020 05:44 PM |                            |
| 3309 | GROMACS                | Bug     | New             | Normal   | -reprod: checkpoint reading bug and general considerations                               |          | 02/27/2020 10:45 PM |                            |
| 3385 | GROMACS                | Bug     | New             | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang                                       |          | 03/04/2020 06:59 PM |                            |
| 3387 | GROMACS                | Bug     | New             | Normal   | Death test bug   |          | 02/20/2020 05:39 PM |                            |
| 3398 | GROMACS                | Bug     | New             | Normal   | Intermittent failure of non-bonded kernels when run using nvprof                         |          | 02/25/2020 12:14 PM |                            |
| 3403 | GROMACS                | Bug     | Resolved        | Normal   | solvation free energy with couple-intramol set to no                                     |          | 12/10/2020 02:45 PM |                            |
| 3405 | GROMACS                | Bug     | Accepted        | Normal   | intermitted OpenCL regressiontest failures   |          | 03/02/2020 11:01 AM |                            |
| 3411 | GROMACS                | Bug     | New             | Normal   | Nightly master release build failure   |          | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3412 | GROMACS                | Bug     | New             | Normal   | Domain decomposition problems with Gromacs >2018   |          | 03/06/2020 04:10 PM |                            |
| 3413 | GROMACS                | Bug     | Feedback wanted | Normal   | COMM Removal Failure in GROMACS 2020.1   |          | 03/12/2020 02:31 PM |                            |
| 3440 | GROMACS                | Bug     | New             | Normal   | Multi-nodes run exits with error with openmpi/4.0.0                                      |          | 03/23/2020 02:10 PM |                            |
| 3442 | GROMACS                | Bug     | Accepted        | Normal   | continuing mdrun with -deffnm and pulling does not work                                  |          | 03/15/2020 08:33 AM |                            |
| 3443 | GROMACS                | Bug     | New             | Normal   | Bonded GPU kernel performance regression with 2020                                       |          | 03/15/2020 08:15 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 |                            |
| 1551 | Support Platforms      | Bug     | Feedback wanted | Normal   | git index.lock issue   |          | 05/31/2017 05:37 PM |                            |
| 1731 | Support Platforms      | Bug     | In Progress     | Normal   | document jenkins configuration and set up means to track changes                         |          | 05/31/2017 06:13 PM |                            |
| 1732 | Support Platforms      | Bug     | New             | Normal   | review and extend jenkins tests setups, coverage   |          | 05/03/2016 05:30 AM |                            |
| 1836 | Support Platforms      | Bug     | New             | Normal   | Support a way to retrigger part of matrix job  |          | 07/22/2017 12:30 AM |                            |
| 1967 | Support Platforms      | Bug     | Resolved        | Normal   | Documentation pages generated by Jenkins do not render properly                          |          | 08/27/2016 02:04 AM |                            |
| 2096 | Support Platforms      | Bug     | New             | Normal   | Redmine internal error with special characters   |          | 05/31/2017 08:48 PM |                            |
| 2149 | Support Platforms      | Bug     | New             | Normal   | gerrit server excessive CPU usage  |          | 04/05/2017 07:25 PM |                            |
| 1536 | TNG trajectory library | Bug     | New             | Normal   | TNG uses incorrect format for size_t on 32bit  |          | 06/28/2014 03:56 AM |                            |

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|------|------------------------|---------|--------------------|----------|--|----------|---------------------|----------------|
| 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 |                |
| 2937 | TNG trajectory library | Bug     | New                | Normal   | tng_num_frames_get reports incorrect num frames  |          | 04/29/2019 11:30 AM |                |
| 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         |
| 895  | GROMACS                | Feature | In Progress        | Normal   | g_rmsf previous frame as reference   |          | 04/29/2013 07:39 PM | future         |
| 907  | GROMACS                | Feature | Accepted           | Normal   | Add tests for verifying installed headers  |          | 03/11/2014 09:15 PM | future         |
| 921  | GROMACS                | Feature | Blocked, need info | Normal   | Default index groups and selections  |          | 07/11/2016 08:27 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         |
| 1028 | GROMACS                | Feature | New                | Normal   | Tool to calculate fraction of native contacts during simulation  |          | 11/01/2012 10:27 PM |                |
| 1083 | GROMACS                | Feature | In Progress        | Normal   | Improve collective error/warning/note handling in mdrun  |          | 07/11/2016 08:21 PM |                |
| 1102 | GROMACS                | Feature | New                | Normal   | Detect incompletely written itp files  |          | 06/19/2014 03:23 PM |                |
| 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 |                |
| 1182 | GROMACS                | Feature | New                | Normal   | improve trajectory writing to support parallel I/O   |          | 05/13/2014 10:42 AM | future         |
| 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 |                |
| 1437 | GROMACS                | Feature | New                | Normal   | Online help formatting improvements  |          | 06/04/2015 09:20 PM | future         |
| 1489 | GROMACS                | Feature | New                | Normal   | Don't solely rely on filename extension  |          | 04/30/2014 05:23 AM |                |
| 1511 | GROMACS                | Feature | Accepted           | Normal   | add PDBx (ie mmcif) support  |          | 10/05/2018 07:14 PM |                |
| 1625 | GROMACS                | Feature | New                | Normal   | Gromacs Python API   |          | 03/02/2019 01:44 AM | future         |
| 1627 | GROMACS                | Feature | In Progress        | Normal   | DPD integrator   |          | 07/11/2016 08:08 PM |                |
| 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 |                |
| 1665 | GROMACS                | Feature | New                | Normal   | improve free energy non-bonded kernel performance  |          | 08/26/2019 03:47 PM | future         |
| 1670 | GROMACS                | Feature | New                | Normal   | create mdrun option checking mini-tool   |          | 06/23/2016 04:06 PM |                |
| 1842 | GROMACS                | Feature | New                | Normal   | Replace XML with JSON  |          | 01/18/2018 05:12 PM |                |
| 1854 | GROMACS                | Feature | New                | Normal   | Remove all cyclic dependencies   |          | 05/25/2017 08:34 AM |                |
| 1867 | GROMACS                | Feature | New                | Normal   | make coupling implementations reversible   |          | 12/02/2015 07:43 AM |                |

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|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------|
| 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 |                |
| 1964 | GROMACS | Feature | Accepted        | Normal   | "pull=no" should not produce warnings about "unknown" pull keywords                              |          | 05/20/2016 02:37 PM |                |
| 1972 | GROMACS | Feature | New             | Normal   | external potential modules for refinement against experimental data                              |          | 08/22/2018 05:03 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 |                |
| 2001 | GROMACS | Feature | New             | Normal   | add MPI info to the mdrun log header   |          | 07/06/2016 05:21 PM |                |
| 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 |                |
| 2060 | GROMACS | Feature | New             | Normal   | Convert enum to enum class   |          | 10/17/2016 05:27 PM |                |
| 2068 | GROMACS | Feature | New             | Normal   | Access to low level classes  |          | 03/02/2019 01:37 AM | future         |
| 2080 | GROMACS | Feature | New             | Normal   | add grompp warning for suitability for domain decomposition                                      |          | 11/23/2016 03:03 PM |                |
| 2111 | GROMACS | Feature | In Progress     | Normal   | Implement Gaussian screening of electrostatics   |          | 02/23/2019 12:33 PM |                |
| 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         |
| 2139 | GROMACS | Feature | New             | Normal   | More precise/explicit documentation conventions  |          | 01/07/2018 11:54 PM |                |
| 2207 | GROMACS | Feature | New             | Normal   | solvent excluded volume of large molecule with periodic boundary condition                       |          | 06/16/2017 10:37 AM |                |
| 2218 | GROMACS | Feature | Feedback wanted | Normal   | A tiny feature: damping for umbrella pull  |          | 08/16/2017 07:20 PM |                |
| 2220 | GROMACS | Feature | New             | Normal   | report relevant env var behaviour to console   |          | 07/31/2017 09:40 PM |                |
| 2226 | GROMACS | Feature | New             | Normal   | Harmonise commands for exit in make_ndx and distance   |          | 08/04/2017 12:24 PM |                |
| 2239 | GROMACS | Feature | New             | Normal   | split libgromacs into base and full  |          | 01/07/2019 01:47 AM |                |
| 2248 | GROMACS | Feature | New             | Normal   | Label all SIMD functions as pure/nodiscard   |          | 02/04/2019 04:49 AM |                |
| 2254 | GROMACS | Feature | Resolved        | Normal   | GPU extensions for Google Tests  |          | 10/06/2020 12:15 PM |                |
| 2289 | GROMACS | Feature | New             | Normal   | gmx spatial add ability to perform over multiple reference structures                            |          | 11/08/2017 12:31 AM |                |
| 2354 | GROMACS | Feature | New             | Normal   | develop configuration file support for control of task layout                                    |          | 09/19/2018 03:01 PM | future         |
| 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         |
| 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 |                |
| 2570 | GROMACS | Feature | New             | Normal   | Better string formatting and printing  |          | 05/02/2019 12:20 PM |                |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------------------|
| 2579 | GROMACS | Feature | New             | Normal   | Add dimensionality option to gmx trjconv -center                               |          | 07/19/2018 04:53 PM | future                     |
| 2581 | GROMACS | Feature | Accepted        | Normal   | User interface for hybrid Monte Carlo  |          | 12/20/2019 12:24 PM | future                     |
| 2585 | GROMACS | Feature | Resolved        | Normal   | Infrastructure supporting external API   |          | 12/11/2019 12:39 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 |                            |
| 2710 | GROMACS | Feature | New             | Normal   | Separate dvdl for each molecule (of couple-moltype) when running FEP           |          | 12/27/2019 04:41 PM | 2021                       |
| 2713 | GROMACS | Feature | New             | Normal   | Constant offset for external electric fields                                   |          | 10/28/2018 12:57 AM |                            |
| 2715 | GROMACS | Feature | New             | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support        |          | 12/27/2019 04:06 PM | future                     |
| 2739 | GROMACS | Feature | New             | Normal   | Parallel continuous tempering and enhanced sampling feature                    |          | 11/13/2018 11:36 PM |                            |
| 2806 | GROMACS | Feature | New             | Normal   | SIMD algorithms for ARM SVE // nobnoded cluster and others                     |          | 12/27/2019 03:59 PM | 2021                       |
| 2840 | GROMACS | Feature | New             | Normal   | Test that functionality does not compile that is not supposed to.              |          | 01/25/2019 02:35 PM | future                     |
| 2860 | GROMACS | Feature | New             | Normal   | Option for outputting min/max coordinates in gmx traj                          |          | 02/08/2019 12:35 AM |                            |
| 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 |                            |
| 2896 | GROMACS | Feature | Feedback wanted | Normal   | Python packaging   |          | 01/16/2020 07:11 PM | 2021-refactoring           |
| 2910 | GROMACS | Feature | New             | Normal   | Mixed scaling for 1-4 interactions   |          | 04/10/2019 10:13 PM |                            |
| 2928 | GROMACS | Feature | New             | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.    |          | 04/16/2019 04:52 PM |                            |
| 2930 | GROMACS | Feature | New             | Normal   | Limited range for reference group detection in cylinder pulling                |          | 04/26/2019 05:17 PM |                            |
| 2931 | GROMACS | Feature | New             | Normal   | Tables in Verlet kernels   |          | 04/29/2019 12:01 PM |                            |
| 2956 | GROMACS | Feature | New             | Normal   | SAXS resolution  |          | 05/17/2019 09:58 AM |                            |
| 2961 | GROMACS | Feature | New             | Normal   | How should Python package find GROMACS resources under various circumstances?  |          | 12/09/2019 10:47 AM |                            |
| 2967 | GROMACS | Feature | New             | Normal   | GPU reallocateDeviceBuffer improvements  |          | 01/23/2020 12:15 PM | 2021-refactoring           |
| 2975 | GROMACS | Feature | New             | Normal   | LJ PME calculations on GPUs  |          | 06/12/2019 01:17 PM |                            |
| 2977 | GROMACS | Feature | New             | Normal   | print DD load balancing improvement  |          | 06/13/2019 10:56 AM |                            |
| 2994 | GROMACS | Feature | New             | Normal   | Data flow topology in gmxapi 2020  |          | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 3021 | GROMACS | Feature | Feedback wanted | Normal   | Completion of docs for GPU developments  |          | 03/02/2020 03:58 PM | 2020.2                     |
| 3030 | GROMACS | Feature | New             | Normal   | RST style guidelines   |          | 07/09/2019 03:38 PM |                            |
| 3032 | GROMACS | Feature | Feedback wanted | Normal   | Clean up dev-manual structure  |          | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3115 | GROMACS | Feature | New             | Normal   | Device stream manager  |          | 10/04/2019 09:00 AM |                            |



| #    | Project           | Tracker | Status          | Priority | Subject   | Assignee | Updated             | Target version             |
|------|-------------------|---------|-----------------|----------|---|----------|---------------------|----------------------------|
| 3126 | GROMACS           | Feature | New             | Normal   | State propagator GPU data manager   |          | 10/09/2019 02:42 PM |                            |
| 3135 | GROMACS           | Feature | New             | Normal   | Make GPU traits into opaque types   |          | 10/14/2019 10:24 AM |                            |
| 3138 | GROMACS           | Feature | New             | Normal   | Improve ensemble support in Context specification.                              |          | 10/15/2019 03:56 PM |                            |
| 3152 | GROMACS           | Feature | New             | Normal   | Infrastructure and patterns for expressing public interfaces                    |          | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3177 | GROMACS           | Feature | New             | Normal   | Spack package management support  |          | 11/06/2019 06:37 PM |                            |
| 3242 | GROMACS           | Feature | New             | Normal   | Please do not remove the -nsteps flag   |          | 03/01/2020 01:59 PM |                            |
| 3277 | GROMACS           | Feature | New             | Normal   | Allow testing feature that is partly implemented                                |          | 12/31/2019 12:44 PM | 2021                       |
| 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                     |
| 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 |
| 3298 | GROMACS           | Feature | New             | Normal   | start early PP work for first dimension of halo exchange                        |          | 03/01/2020 01:36 PM |                            |
| 3307 | GROMACS           | Feature | New             | Normal   | General interface for communication between simulation ranks                    |          | 01/22/2020 03:22 PM | 2021-refactoring           |
| 3311 | GROMACS           | Feature | In Progress     | Normal   | GPU infrastructure development  |          | 03/20/2020 09:54 AM | 2021-refactoring           |
| 3328 | GROMACS           | Feature | New             | Normal   | Testing framework for task assignment   |          | 01/22/2020 09:48 AM | 2021-refactoring           |
| 3332 | GROMACS           | Feature | New             | Normal   | gmx helixorient doesn't have a -tu option to change time unit                   |          | 01/22/2020 11:57 AM |                            |
| 3362 | GROMACS           | Feature | New             | Normal   | gmx traj: add an option to plot each component in a separate file               |          | 01/29/2020 06:18 PM |                            |
| 3369 | GROMACS           | Feature | New             | Normal   | Add quote about "the truth"   |          | 02/05/2020 05:08 PM |                            |
| 3374 | GROMACS           | Feature | New             | Normal   | SimulationInput abstraction   |          | 03/03/2020 05:32 PM | 2021-refactoring           |
| 3378 | GROMACS           | Feature | New             | Normal   | genion usage without stdin (facilitates use in gmx python api)                  |          | 02/13/2020 12:04 PM |                            |
| 3379 | GROMACS           | Feature | New             | Normal   | C++ API for simulation input and output   |          | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3395 | GROMACS           | Feature | Feedback wanted | Normal   | Consider scripted composition of Dockerfiles                                    |          | 03/16/2020 12:16 PM |                            |
| 3401 | GROMACS           | Feature | New             | Normal   | Policy and procedure for installed headers (public API)                         |          | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3402 | GROMACS           | Feature | New             | Normal   | Clarify distinction between public API documentation and developer docs.        |          | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3439 | GROMACS           | Feature | New             | Normal   | Optimize successive simulation segments   |          | 03/11/2020 01:42 PM |                            |
| 687  | Support Platforms | Feature | New             | Normal   | Add content on the front page   |          | 09/02/2019 01:08 PM |                            |
| 987  | Support Platforms | Feature | New             | Normal   | Feature wishlist should be moved to Redmine                                     |          | 08/03/2012 12:22 PM |                            |
| 1601 | Support Platforms | Feature | New             | Normal   | use Git for Jenkins Config  |          | 05/24/2015 10:59 AM |                            |
| 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 |                            |

| #    | Project                | Tracker | Status             | Priority | Subject   | Assignee | Updated             | Target version |
|------|------------------------|---------|--------------------|----------|---|----------|---------------------|----------------|
| 1197 | TNG trajectory library | Feature | New                | Normal   | Rework the molecule descriptions                                    |          | 03/18/2013 04:16 PM | version 2      |
| 1202 | TNG trajectory library | Feature | New                | Normal   | Other hash types  |          | 06/25/2013 10:02 PM | version 2      |
| 652  | GROMACS                | Task    | Blocked, need info | Normal   | Change selection method implementation to use C++                   |          | 04/23/2017 08:05 PM | future         |
| 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 |                |
| 701  | GROMACS                | Task    | New                | Normal   | Add symbol visibility macros  |          | 03/02/2019 01:46 AM | future         |
| 838  | GROMACS                | Task    | New                | Normal   | Improve generic error reporting routines                            |          | 07/11/2016 08:29 PM |                |
| 909  | GROMACS                | Task    | New                | Normal   | Reimplement displacement calculation module                         |          | 07/14/2014 11:30 AM | future         |
| 986  | GROMACS                | Task    | New                | Normal   | Handling C++ out-of-memory errors                                   |          | 12/24/2014 08:42 PM | future         |
| 988  | GROMACS                | Task    | New                | Normal   | Definition of "public API"  |          | 08/28/2019 02:50 PM | future         |
| 1017 | GROMACS                | Task    | New                | Normal   | C++ Vector/Matrix classes   |          | 07/11/2016 08:23 PM |                |
| 1140 | GROMACS                | Task    | New                | Normal   | Class design for passing options and data                           |          | 07/11/2016 08:19 PM |                |
| 1170 | GROMACS                | Task    | New                | Normal   | mdlib reorganization  |          | 11/17/2016 03:47 PM | future         |
| 1523 | GROMACS                | Task    | New                | Normal   | add missing code-paths to CUDA emulation kernel                     |          | 07/11/2016 08:09 PM |                |
| 1587 | GROMACS                | Task    | New                | Normal   | improve the configurability of regression tests                     |          | 12/20/2019 12:02 PM | 2021           |
| 1729 | GROMACS                | Task    | New                | Normal   | Resolve whether and how to resolve "state" variables stored in .tpr |          | 05/13/2015 10:48 AM | future         |
| 1745 | GROMACS                | Task    | New                | Normal   | Moving to C++11 after Gromacs-5.1                                   |          | 06/01/2016 03:01 PM |                |
| 1768 | GROMACS                | Task    | New                | Normal   | decide future of command-line options vs env vars                   |          | 11/03/2016 05:51 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 |                |
| 1852 | GROMACS                | Task    | New                | Normal   | Remove group scheme   |          | 03/03/2020 09:03 PM | future         |
| 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 |                |
| 1876 | GROMACS                | Task    | New                | Normal   | Reorganize vector input passed to core MD routines                  |          | 06/01/2016 01:59 PM | future         |
| 1925 | GROMACS                | Task    | In Progress        | Normal   | remove concept of unilateral global communication                   |          | 12/29/2019 10:35 AM | 2021           |
| 1936 | GROMACS                | Task    | New                | Normal   | treat default-able mdp fields as strings                            |          | 04/02/2016 10:32 PM | future         |
| 1971 | GROMACS                | Task    | New                | Normal   | Removing buggy features vs. keeping workflows                       |          | 01/19/2018 01:36 PM | future         |
| 1973 | GROMACS                | Task    | New                | Normal   | OpenCL implementation wish list                                     |          | 05/27/2016 03:42 PM |                |
| 2003 | GROMACS                | Task    | New                | Normal   | reconsider various simd flags                                       |          | 07/07/2016 11:23 PM |                |
| 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 |                |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee | Updated             | Target version |
|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------|
| 2035 | GROMACS | Task    | New             | Normal   | A common trajectory analysis data exchange format                                      |          | 03/15/2017 05:46 PM | future         |
| 2048 | GROMACS | Task    | New             | Normal   | C++11: CUDA dependency on general headers  |          | 09/07/2016 10:30 PM |                |
| 2053 | GROMACS | Task    | New             | Normal   | refine notation in GPU code  |          | 12/20/2019 01:04 PM | 2021           |
| 2059 | GROMACS | Task    | In Progress     | Normal   | Separate different types of data in t_state  |          | 12/27/2019 04:42 PM | 2021           |
| 2089 | GROMACS | Task    | New             | Normal   | Encourage code review  |          | 01/10/2017 12:03 AM |                |
| 2092 | GROMACS | Task    | New             | Normal   | Tests running on GPU, and hardware assignment  |          | 12/19/2017 05:27 PM | future         |
| 2115 | GROMACS | Task    | New             | Normal   | trjconv does too many things, and combinations of them work poorly                     |          | 10/02/2018 09:04 AM |                |
| 2158 | GROMACS | Task    | New             | Normal   | consider adding post-submit test that runs PME with 2xNN kernels                       |          | 04/19/2017 08:04 PM |                |
| 2166 | GROMACS | Task    | Accepted        | Normal   | gmx trjconv functionality should check for mismatch between the tpr and the trajectory |          | 05/05/2017 04:32 PM |                |
| 2168 | GROMACS | Task    | Feedback wanted | Normal   | Design for multiple comparisons against same test reference data                       |          | 05/08/2017 02:45 PM | future         |
| 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 |                |
| 2185 | GROMACS | Task    | New             | Normal   | add docs on MPI + CUDA w/wo MPS  |          | 05/24/2017 05:17 PM |                |
| 2221 | GROMACS | Task    | New             | Normal   | Avoid preprocessor for SIMD functions  |          | 02/21/2018 01:43 PM |                |
| 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         |
| 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           |
| 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         |
| 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 |                |
| 2382 | GROMACS | Task    | New             | Normal   | Simplify Doxygen guidelines  |          | 01/13/2018 12:40 AM |                |
| 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 |                |
| 2435 | GROMACS | Task    | New             | Normal   | identify and note about/tune task offload in GPU-bound runs                            |          | 03/02/2018 04:08 PM |                |
| 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 |                |
| 2448 | GROMACS | Task    | Accepted        | Normal   | should mdrun -multidir permit only one directory?                                      |          | 03/21/2018 12:10 PM |                |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee | Updated             | Target version             |
|------|---------|---------|-------------|----------|---|----------|---------------------|----------------------------|
| 2456 | GROMACS | Task    | New         | Normal   | Add a pull module external potential tests  |          | 03/15/2018 03:02 PM |                            |
| 2462 | GROMACS | Task    | New         | Normal   | consider adding STL misuse tests  |          | 03/23/2018 01:23 AM |                            |
| 2464 | GROMACS | Task    | New         | Normal   | GPU performance goals overview  |          | 03/26/2018 10:42 AM |                            |
| 2469 | GROMACS | Task    | New         | Normal   | implement GPU timer reduction for reporting                                       |          | 03/27/2018 05:08 PM |                            |
| 2475 | GROMACS | Task    | New         | Normal   | make OpenCL 1st class-citizen in the build system                                 |          | 12/20/2019 12:14 PM | 2021                       |
| 2488 | GROMACS | Task    | New         | Normal   | use MPI non-blocking collectives to overlap pull comm                             |          | 04/25/2018 04:19 PM |                            |
| 2498 | GROMACS | Task    | New         | Normal   | OpenCL memory pinning/mapping   |          | 12/20/2019 12:18 PM | future                     |
| 2514 | GROMACS | Task    | New         | Normal   | PME OpenCL reductions with intrinsics   |          | 05/31/2018 12:27 AM | future                     |
| 2518 | GROMACS | Task    | New         | Normal   | redesign task-assignment code for OpenCL  |          | 12/20/2019 12:19 PM | future                     |
| 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 |                            |
| 2522 | GROMACS | Task    | Resolved    | Normal   | OpenCL context duplication  |          | 03/11/2020 04:15 PM | future                     |
| 2524 | GROMACS | Task    | New         | Normal   | struct alignment/packing for OpenCL host & device code                            |          | 12/20/2019 12:20 PM | future                     |
| 2527 | GROMACS | Task    | New         | Normal   | Rename GpuEventSynchronizer to something more fitting (after merge in 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                     |
| 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 |                            |
| 2608 | GROMACS | Task    | New         | Normal   | Remove code duplication between OpenCL and CUDA                                   |          | 09/24/2018 12:47 PM |                            |
| 2616 | GROMACS | Task    | New         | Normal   | Model for MD state  |          | 09/14/2018 05:12 PM |                            |
| 2650 | GROMACS | Task    | New         | Normal   | revise OpenCL stack recommendations   |          | 12/31/2018 11:19 AM | future                     |
| 2671 | GROMACS | Task    | New         | Normal   | replace constants like M_PI   |          | 12/20/2019 01:17 PM | future                     |
| 2672 | GROMACS | Task    | New         | Normal   | check & document execution width requirements in OpenCL                           |          | 12/31/2018 11:20 AM | future                     |
| 2674 | GROMACS | Task    | Accepted    | Normal   | Improve domain decomposition for bilayer systems                                  |          | 12/07/2018 04:03 PM | future                     |
| 2675 | GROMACS | Task    | In Progress | Normal   | bonded CUDA offload task  |          | 02/12/2020 05:54 PM | 2021                       |
| 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                       |
| 2697 | GROMACS | Task    | New         | Normal   | improve FFT library flavor/version reporting                                      |          | 12/27/2019 04:40 PM | future                     |
| 2698 | GROMACS | Task    | In Progress | Normal   | gmxapi documentation integration  |          | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 2699 | GROMACS | Task    | New         | Normal   | Test POWER9   |          | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 2706 | GROMACS | Task    | Accepted    | Normal   | Rework classic QM/MM interface  |          | 12/02/2019 01:45 PM | 2021-infrastructure-stable |
| 2756 | GROMACS | Task    | In Progress | Normal   | gmxapi integration testing  |          | 01/16/2020 05:12 PM | 2021-refactoring           |

| #    | Project | Tracker | Status      | Priority | Subject  | Assignee | Updated             | Target version             |
|------|---------|---------|-------------|----------|--|----------|---------------------|----------------------------|
| 2770 | GROMACS | Task    | New         | Normal   | change branch maintenance policy   |          | 01/16/2020 05:09 PM | 2021                       |
| 2771 | GROMACS | Task    | New         | Normal   | Size independent Hessian for normal mode analysis  |          | 12/28/2019 10:50 AM | future                     |
| 2773 | GROMACS | Task    | New         | Normal   | improve GPU error handling and make such handling uniform across modules                   |          | 12/20/2019 01:09 PM | 2021                       |
| 2787 | GROMACS | Task    | New         | Normal   | allow passing flags to allocateDeviceBuffer  |          | 12/03/2018 01:54 PM |                            |
| 2795 | GROMACS | Task    | New         | Normal   | Incorporate regressiontests into core gromacs  |          | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2835 | GROMACS | Task    | New         | Normal   | Matrix class constraint to upper or lower triangle   |          | 02/07/2019 02:44 PM |                            |
| 2839 | GROMACS | Task    | New         | Normal   | make module and file naming consistent   |          | 01/16/2020 05:11 PM | 2021                       |
| 2855 | GROMACS | Task    | New         | Normal   | Allow compiling GROMACS without C compiler   |          | 01/10/2020 12:06 PM |                            |
| 2857 | GROMACS | Task    | New         | Normal   | Clarify recommended function specifies (constexpr, noexcept, pure)                         |          | 02/04/2019 04:48 AM |                            |
| 2859 | GROMACS | Task    | Resolved    | Normal   | Change ArrayRef iterator type from pointer to std::iterator                                |          | 06/26/2020 06:15 PM |                            |
| 2863 | GROMACS | Task    | New         | Normal   | improve PBC handling   |          | 03/11/2019 04:28 PM |                            |
| 2905 | GROMACS | Task    | New         | Normal   | Add a Jenkins configuration with std library assert  |          | 08/24/2019 05:22 PM |                            |
| 2909 | GROMACS | Task    | New         | Normal   | consider implementing mechanisms to ensure pair lists are not used past their max lifetime |          | 04/03/2019 05:14 PM |                            |
| 2919 | GROMACS | Task    | New         | Normal   | C++ style guidelines for namespace use   |          | 04/15/2019 01:21 PM |                            |
| 2933 | GROMACS | Task    | New         | Normal   | Convert walls to a ForceProvider   |          | 04/25/2019 02:43 PM |                            |
| 2936 | GROMACS | Task    | New         | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types       |          | 02/05/2020 03:57 PM | 2021                       |
| 2947 | GROMACS | Task    | Accepted    | Normal   | make an end to end test for membed   |          | 09/24/2019 03:22 PM | future                     |
| 2965 | GROMACS | Task    | In Progress | Normal   | Performance of GPU direct communications   |          | 02/14/2020 12:38 PM | 2021                       |
| 2976 | GROMACS | Task    | New         | Normal   | Basic math for Multidimensional arrays   |          | 12/27/2019 04:37 PM | 2021                       |
| 2983 | GROMACS | Task    | New         | Normal   | better suited data-types for bonded GPU kernels  |          | 07/11/2019 04:32 PM |                            |
| 2992 | GROMACS | Task    | New         | Normal   | Split hw_opt in const user options and dynamic settings                                    |          | 12/27/2019 04:31 PM | future                     |
| 2997 | GROMACS | Task    | New         | Normal   | improve performance of alchemical free energy calculations                                 |          | 12/27/2019 04:31 PM | 2021                       |
| 2998 | GROMACS | Task    | Resolved    | Normal   | Update Python detection  |          | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 2999 | GROMACS | Task    | New         | Normal   | Move all logging in core library and tools to use MDLogger                                 |          | 09/06/2019 02:36 PM | 2021-infrastructure-stable |
| 3001 | GROMACS | Task    | New         | Normal   | explore simplifying virial and shift force reduction                                       |          | 12/27/2019 04:30 PM | 2021                       |
| 3002 | GROMACS | Task    | New         | Normal   | consider splitting bonded work into local/nonlocal   |          | 06/25/2019 04:06 PM |                            |
| 3003 | GROMACS | Task    | New         | Normal   | implement heuristic fallback to CPU when there is too little work for GPU offload          |          | 06/25/2019 04:10 PM |                            |
| 3004 | GROMACS | Task    | New         | Normal   | Move trajectory analysis logging to MDLogger   |          | 06/26/2019 09:59 AM |                            |
| 3005 | GROMACS | Task    | New         | Normal   | Move logging in gmx preprocess to MDLogger   |          | 06/26/2019 10:01 AM |                            |
| 3008 | GROMACS | Task    | New         | Normal   | verify block size choice of CUDA bonded kernel   |          | 12/27/2019 04:30 PM | 2021                       |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|----------|---------------------|----------------------------|
| 3010 | GROMACS | Task    | In Progress     | Normal   | upgrade OpenCL stack on bs-gpu01  |          | 12/20/2019 08:25 AM | 2021-infrastructure-stable |
| 3013 | GROMACS | Task    | New             | Normal   | Extend logging levels in MDLogger   |          | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task    | In Progress     | Normal   | gmxapi example Python scripts   |          | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 3015 | GROMACS | Task    | New             | Normal   | Create central log handle for calls to gmx_fatal  |          | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3016 | GROMACS | Task    | New             | Normal   | intermittent failure of essentialdynamics test  |          | 07/18/2019 05:23 PM |                            |
| 3031 | GROMACS | Task    | New             | Normal   | evaluate the impact of particle order on PME  |          | 12/27/2019 04:29 PM | 2021                       |
| 3033 | GROMACS | Task    | In Progress     | Normal   | Clean up and modernize googletest bundling and usage  |          | 01/16/2020 04:50 PM | 2021-refactoring           |
| 3040 | GROMACS | Task    | New             | Normal   | Refactor Restraint module   |          | 07/18/2019 03:59 PM |                            |
| 3041 | GROMACS | Task    | Resolved        | Normal   | Remove workaround for gcc bug 58265   |          | 06/19/2020 04:45 PM |                            |
| 3047 | GROMACS | Task    | Feedback wanted | Normal   | Set required versions for GROMACS 2021  |          | 02/20/2020 11:42 AM |                            |
| 3062 | GROMACS | Task    | New             | Normal   | add twin cut-off mdrun test   |          | 12/27/2019 04:22 PM | 2021                       |
| 3064 | GROMACS | Task    | New             | Normal   | add test for perturbed bonded forces  |          | 12/27/2019 04:22 PM | 2021                       |
| 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 |                            |
| 3078 | GROMACS | Task    | New             | Normal   | Allow MD modules to register energy output fields themselves  |          | 09/06/2019 11:36 AM |                            |
| 3104 | GROMACS | Task    | New             | Normal   | implement GPU DD cycle counting   |          | 12/27/2019 04:21 PM | 2021                       |
| 3105 | GROMACS | Task    | New             | Normal   | implement GPU PME/PP comm cycle counting  |          | 12/27/2019 04:20 PM | 2021                       |
| 3119 | GROMACS | Task    | New             | Normal   | clang-tidy coverage of parallelizaton codepaths   |          | 12/27/2019 04:20 PM | 2021                       |
| 3123 | GROMACS | Task    | New             | Normal   | address sanitizer coverage of parallelization code-paths  |          | 10/05/2019 12:32 AM |                            |
| 3132 | GROMACS | Task    | New             | Normal   | gmxapi testing support tools  |          | 10/31/2019 03:35 PM |                            |
| 3171 | GROMACS | Task    | New             | Normal   | schedule CPU H2D force contribution in separate stream  |          | 12/20/2019 08:33 AM | 2021-infrastructure-stable |
| 3181 | GROMACS | Task    | New             | Normal   | consolidate task assignment and workload data initialization  |          | 10/28/2019 02:53 PM |                            |
| 3183 | GROMACS | Task    | Accepted        | Normal   | enable bonded interactions on GPU   |          | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 3185 | GROMACS | Task    | New             | Normal   | Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels. |          | 10/30/2019 11:18 AM |                            |
| 3186 | GROMACS | Task    | In Progress     | Normal   | Update Constant/Variable naming in the PME GPU kernels.   |          | 10/30/2019 11:23 AM |                            |
| 3187 | GROMACS | Task    | New             | Normal   | Template updated PME kernels using threads per atom   |          | 10/30/2019 11:33 AM |                            |
| 3194 | GROMACS | Task    | New             | Normal   | consider passing GPU dependency list to both dependency producers and consumers                           |          | 11/01/2019 07:10 PM |                            |
| 3201 | GROMACS | Task    | In Progress     | Normal   | Convert mdp parameters to key value tree  |          | 11/06/2019 06:06 PM |                            |
| 3212 | GROMACS | Task    | New             | Normal   | Update regression tests for new kernel flavours   |          | 11/21/2019 11:50 AM |                            |
| 3220 | GROMACS | Task    | New             | Normal   | change rolling pruning scheduling with GPU update   |          | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3224 | GROMACS | Task    | New             | Normal   | add regression test case large enough to miscalculated GPU grid launch cases                              |          | 12/20/2019 01:18 PM | 2021                       |

| #    | Project           | Tracker | Status      | Priority | Subject   | Assignee | Updated             | Target version             |
|------|-------------------|---------|-------------|----------|---|----------|---------------------|----------------------------|
| 3229 | GROMACS           | Task    | New         | Normal   | Move checkpointing to the beginning of the MD step  |          | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3252 | GROMACS           | Task    | New         | Normal   | Remove support for 32 bit architectures   |          | 03/01/2020 02:05 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 |                            |
| 3255 | GROMACS           | Task    | New         | Normal   | Move benchmarking options from mdrun to a dedicated tool                                      |          | 12/19/2019 01:21 PM |                            |
| 3256 | GROMACS           | Task    | New         | Normal   | Remove -nsteps option from mdrun  |          | 12/19/2019 12:12 PM |                            |
| 3267 | GROMACS           | Task    | New         | Normal   | Document tools  |          | 12/26/2019 03:20 PM | future                     |
| 3268 | GROMACS           | Task    | New         | Normal   | add more Intel driver recommendations   |          | 12/26/2019 04:39 PM |                            |
| 3271 | GROMACS           | Task    | Resolved    | Normal   | Adopt PEP-518 for Python package build system configuration.                                  |          | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3287 | GROMACS           | Task    | New         | Normal   | Deprecate make_ndx, use select instead  |          | 01/23/2020 01:16 PM |                            |
| 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 |
| 3300 | GROMACS           | Task    | New         | Normal   | Abandon docs/OpenCLTODOList.txt?  |          | 01/15/2020 02:46 PM |                            |
| 3308 | GROMACS           | Task    | New         | Normal   | GPU update-constraints: Cycle counting for GPU launches                                       |          | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3324 | GROMACS           | Task    | New         | Normal   | Rework CMake handling of GPU code   |          | 01/22/2020 09:52 AM | 2021-refactoring           |
| 3325 | GROMACS           | Task    | New         | Normal   | Allow complete re-initialization of a simulation  |          | 01/29/2020 05:13 PM | 2021-refactoring           |
| 3326 | GROMACS           | Task    | New         | Normal   | Allow changing task assignment  |          | 01/22/2020 09:44 AM | 2021-refactoring           |
| 3327 | GROMACS           | Task    | New         | Normal   | Refactor workload flags   |          | 01/22/2020 09:45 AM | 2021-refactoring           |
| 3329 | GROMACS           | Task    | New         | Normal   | Extend energy comparison testing framework  |          | 01/22/2020 09:51 AM | 2021-refactoring           |
| 3330 | GROMACS           | Task    | New         | Normal   | Compile list of codepaths for testing task assignment   |          | 01/22/2020 10:03 AM | 2021-refactoring           |
| 3353 | GROMACS           | Task    | New         | Normal   | Document gmx densmap output   |          | 01/23/2020 12:52 PM |                            |
| 3356 | GROMACS           | Task    | New         | Normal   | Expose setting of random seed to API  |          | 01/29/2020 06:16 PM | 2021                       |
| 3357 | GROMACS           | Task    | New         | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs                            |          | 03/04/2020 11:25 AM |                            |
| 3360 | GROMACS           | Task    | New         | Normal   | investigate the future of DD dynamic load balancing with GPU offload                          |          | 01/29/2020 11:23 AM |                            |
| 3366 | GROMACS           | Task    | New         | Normal   | Enforce compability of MdModules  |          | 02/28/2020 11:20 AM |                            |
| 3382 | GROMACS           | Task    | Accepted    | Normal   | Split up t_inputrec   |          | 02/17/2020 05:28 PM |                            |
| 1309 | Support Platforms | Task    | New         | Normal   | Jenkins verification improvements   |          | 06/01/2017 02:34 PM |                            |
| 1508 | Support Platforms | Task    | New         | Normal   | Update master Jenkins build configurations  |          | 06/28/2014 03:59 AM |                            |
| 1815 | Support Platforms | Task    | In Progress | Normal   | implement and execute plan for new releng machinery   |          | 10/15/2016 05:37 PM |                            |
| 2851 | Support Platforms | Task    | New         | Normal   | uninstall redmine checklist plugin  |          | 01/30/2019 03:33 PM |                            |
| 1476 | GROMACS           | Bug     | New         | Low      | Odd behavior with verlet-buffer-drift   |          | 05/25/2016 01:45 AM | future                     |
| 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 |
|------|---------|---------|--------------------|----------|---|----------|---------------------|----------------|
| 1827 | GROMACS | Bug     | New                | Low      | cmake multi-configuration generator support partly broken   |          | 12/11/2017 05:20 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         |
| 1985 | GROMACS | Bug     | Fix uploaded       | Low      | CUDA build system refactoring awaiting review   |          | 12/20/2019 12:07 PM | 2021           |
| 2211 | GROMACS | Bug     | New                | Low      | gmx writes normal output to stderr  |          | 03/05/2018 02:00 PM | future         |
| 2217 | GROMACS | Bug     | New                | Low      | GPU emulation and separate PME ranks doesn't work properly  |          | 12/12/2017 11:50 AM |                |
| 2241 | GROMACS | Bug     | New                | Low      | refdata can segfault when reading   |          | 09/07/2017 11:57 AM |                |
| 2252 | GROMACS | Bug     | New                | Low      | Memory allocation failures with large page sizes during PME tuning  |          | 12/14/2017 04:27 AM |                |
| 2360 | GROMACS | Bug     | New                | Low      | error at counter reset with PME-only rank   |          | 01/05/2018 12:43 PM | future         |
| 2373 | GROMACS | Bug     | New                | Low      | gmx -nice can't work  |          | 01/04/2018 11:17 AM |                |
| 2380 | GROMACS | Bug     | New                | Low      | cycle counter issues with separate PME rank + GPUs  |          | 01/16/2018 10:21 PM |                |
| 2468 | GROMACS | Bug     | New                | Low      | incorrect GPU timing reported with OpenCL and domain decomposition  |          | 12/17/2018 01:28 PM | future         |
| 2555 | GROMACS | Bug     | New                | Low      | building GROMACS 2018.2   |          | 07/03/2018 11:41 PM |                |
| 2568 | GROMACS | Bug     | New                | Low      | gmx editconf -rotate does not rotate the box  |          | 07/10/2018 10:27 AM | future         |
| 2602 | GROMACS | Bug     | New                | Low      | build information gets outdated if build tree is reused   |          | 08/13/2018 09:04 PM |                |
| 2852 | GROMACS | Bug     | New                | Low      | the in-tree regressiontest download can get out of sync with code   |          | 01/30/2019 03:58 PM |                |
| 3202 | GROMACS | Bug     | New                | Low      | gmx solvate fails to overwrite topology file  |          | 11/13/2019 02:44 PM |                |
| 3310 | GROMACS | Bug     | Blocked, need info | Low      | Thread affinity on Mac OS   |          | 02/27/2020 11:10 PM |                |
| 720  | GROMACS | Feature | Accepted           | Low      | permit pdb2gmx to choose a kind of HIS based on proton position   |          | 11/17/2016 03:51 PM | future         |
| 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 |                |
| 1104 | GROMACS | Feature | New                | Low      | Implement dihedral restraints   |          | 02/06/2013 07:04 PM | future         |
| 1120 | GROMACS | Feature | New                | Low      | Make build work with multi-configuration generators   |          | 06/03/2014 03:04 PM | future         |
| 1165 | GROMACS | Feature | Accepted           | Low      | Multi-SIMD binaries   |          | 12/20/2019 12:00 PM | future         |
| 1602 | GROMACS | Feature | New                | Low      | gmx order S per slice along all 3 axes  |          | 09/22/2014 07:25 AM |                |
| 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         |
| 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 |                |
| 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         |
| 1966 | GROMACS | Feature | New                | Low      | Hydrogen mass repartitioning  |          | 05/25/2016 06:04 PM | future         |



| #    | 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                     |
| 2056 | GROMACS                | Feature | New          | Low      | rename "gmx select"   |          | 10/03/2016 08:24 PM |                            |
| 2097 | GROMACS                | Feature | New          | Low      | Move output of dhdl file entirely toedr, rather than having a separate text dhdl file |          | 01/05/2017 05:21 PM | future                     |
| 2101 | GROMACS                | Feature | New          | Low      | warninp could print the offending line, as well as its number                         |          | 01/20/2017 03:06 PM |                            |
| 2118 | GROMACS                | Feature | New          | Low      | More verbose comments requested in header of gmx distance -oxyz                       |          | 02/08/2017 05:46 AM |                            |
| 2194 | GROMACS                | Feature | Accepted     | Low      | xvg output requested as an output option in place of xpm files                        |          | 05/31/2017 04:26 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                     |
| 2622 | GROMACS                | Feature | New          | Low      | Reduce severity of Berendsen warning  |          | 08/23/2018 11:16 PM | future                     |
| 2643 | GROMACS                | Feature | New          | Low      | mdp options and/or docs for anisotropic aspects of implementations                    |          | 09/12/2018 02:23 PM |                            |
| 2761 | GROMACS                | Feature | New          | Low      | lincs-order 4 is too conservative for some force fields                               |          | 11/16/2018 09:55 AM |                            |
| 2846 | GROMACS                | Feature | New          | Low      | Set rpath in FindLibStdCpp.cmake  |          | 02/02/2019 08:09 AM |                            |
| 3020 | GROMACS                | Feature | New          | Low      | modernize DeviceBuffer and GPU memory management                                      |          | 08/13/2019 06:01 PM |                            |
| 3045 | GROMACS                | Feature | New          | Low      | Option to remove v-sites in trjconv?  |          | 07/19/2019 04:42 PM |                            |
| 2180 | Support Platforms      | Feature | Fix uploaded | Low      | releng matrices would work better with a hint for execution                           |          | 05/19/2017 01:02 AM |                            |
| 1206 | TNG trajectory library | Feature | New          | Low      | XTC Compression   |          | 10/25/2013 03:43 PM | version 2                  |
| 1530 | GROMACS                | Task    | New          | Low      | Offer binary downloads  |          | 06/29/2014 02:58 PM |                            |
| 1785 | GROMACS                | Task    | New          | Low      | no pV term written to energy file when pressure coupling is anisotropic               |          | 07/26/2015 01:47 PM | future                     |
| 1879 | GROMACS                | Task    | In Progress  | Low      | make the GROMACS OpenCL kernel work on Gallium  |          | 11/30/2018 05:46 PM | future                     |
| 1907 | GROMACS                | Task    | Accepted     | Low      | keeping compile- and run-time CPU/arch detection consistent                           |          | 08/01/2016 10:09 PM |                            |
| 2055 | GROMACS                | Task    | New          | Low      | Wiki registration is broken   |          | 01/20/2017 11:31 AM |                            |
| 2069 | GROMACS                | Task    | New          | Low      | Simple thread-parallelism inside routines   |          | 11/09/2016 06:06 PM |                            |
| 2084 | GROMACS                | Task    | New          | Low      | MPI and stderr/log output   |          | 11/28/2016 06:37 PM |                            |
| 2133 | GROMACS                | Task    | New          | Low      | gmx traj needs reform   |          | 03/07/2017 02:02 PM |                            |
| 2182 | GROMACS                | Task    | New          | Low      | de-duplicate code in densorder and hydorder   |          | 05/16/2017 11:29 AM |                            |
| 2240 | GROMACS                | Task    | Accepted     | Low      | GPU emulation mode support for PME missing  |          | 09/16/2017 10:02 PM |                            |
| 2341 | GROMACS                | Task    | New          | Low      | assess the state of building and using GROMACS on Windows                             |          | 07/29/2019 11:09 PM | future                     |
| 2463 | GROMACS                | Task    | New          | Low      | PME GPU decomposition   |          | 03/26/2018 10:42 AM |                            |
| 2478 | GROMACS                | Task    | New          | Low      | avoid use of getenv in static initialization  |          | 04/13/2018 11:57 AM |                            |
| 2481 | GROMACS                | Task    | New          | Low      | Update gmx report-methods to write more method information                            |          | 12/02/2019 01:22 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status      | Priority | Subject  | Assignee | Updated             | Target version |
|------|---------|---------|-------------|----------|--|----------|---------------------|----------------|
| 2496 | GROMACS | Task    | New         | Low      | find system xdr properly   |          | 05/02/2018 02:19 PM |                |
| 2531 | GROMACS | Task    | New         | Low      | Consider optimizing tabulated data access on GPU                             |          | 07/30/2018 12:31 PM |                |
| 2632 | GROMACS | Task    | New         | Low      | make sure cmake defines proper hwloc versionc with cross-compilation enabled |          | 12/03/2018 01:35 PM | future         |
| 2670 | GROMACS | Task    | New         | Low      | remove old/backward compatibility OpenCL support from releng                 |          | 10/04/2018 06:06 PM |                |
| 2695 | GROMACS | Task    | New         | Low      | bonded GPU module timing   |          | 12/27/2019 04:40 PM | 2021           |
| 2758 | GROMACS | Task    | New         | Low      | Modernize genconf  |          | 11/15/2018 07:38 AM | future         |
| 2796 | GROMACS | Task    | New         | Low      | clarify what mdrun -cpt means  |          | 01/03/2019 02:09 PM |                |
| 2898 | GROMACS | Task    | New         | Low      | Naming common variables  |          | 03/26/2019 11:46 PM |                |
| 2988 | GROMACS | Task    | In Progress | Low      | clean up and refactor code to modern standards                               |          | 12/27/2019 04:37 PM | future         |

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