

## Issues

| #    | Project | Tracker | Status             | Priority | Subject   | Assignee       | Updated             | Target version             |
|------|---------|---------|--------------------|----------|---|----------------|---------------------|----------------------------|
| 2628 | GROMACS | Bug     | Resolved           | Normal   | GMXRC removes trailing colon from existing MANPATH  |                | 11/02/2020 11:45 AM |                            |
| 3219 | GROMACS | Bug     | Resolved           | Normal   | MANPATH setting is fragile  |                | 11/02/2020 11:45 AM |                            |
| 3444 | GROMACS | Bug     | Resolved           | Normal   | do_dssp does not work(gmx 2020 and 2020.1)  | Christian Blau | 06/10/2020 02:45 PM | 2020.2                     |
| 3380 | GROMACS | Bug     | Resolved           | Low      | IBM VSX checks fail with gcc-10   | Erik Lindahl   | 04/30/2020 01:30 PM | 2020.2                     |
| 3403 | GROMACS | Bug     | Resolved           | Normal   | solvation free energy with couple-intramol set to no  |                | 04/17/2020 04:00 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 |                            |
| 3440 | GROMACS | Bug     | New                | Normal   | Multi-nodes run exits with error with openmpi/4.0.0   |                | 03/23/2020 02:10 PM |                            |
| 3408 | GROMACS | Bug     | Fix uploaded       | Normal   | Gmxapi* tests segfault in rpmbuild  | Eric Irrgang   | 03/23/2020 01:27 PM | 2020.2                     |
| 3441 | GROMACS | Bug     | Resolved           | Normal   | Ewald surface-epsilon is incorrect  | Berk Hess      | 03/18/2020 11:15 PM | 2020.2                     |
| 3443 | GROMACS | Bug     | New                | Normal   | Bonded GPU kernel performance regression with 2020  |                | 03/15/2020 08:15 PM |                            |
| 3442 | GROMACS | Bug     | Accepted           | Normal   | continuing mdrun with -deffnm and pulling does not work   |                | 03/15/2020 08:33 AM |                            |
| 3413 | GROMACS | Bug     | Feedback wanted    | Normal   | COMM Removal Failure in GROMACS 2020.1  |                | 03/12/2020 02:31 PM |                            |
| 3412 | GROMACS | Bug     | New                | Normal   | Domain decomposition problems with Gromacs >2018  |                | 03/06/2020 04:10 PM |                            |
| 3411 | GROMACS | Bug     | New                | Normal   | Nightly master release build failure  |                | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3385 | GROMACS | Bug     | New                | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang  |                | 03/04/2020 06:59 PM |                            |
| 2958 | GROMACS | Bug     | New                | Normal   | Compiling master (to become 2020) using CUDA 9.0  |                | 03/02/2020 03:57 PM | 2020.2                     |
| 3405 | GROMACS | Bug     | Accepted           | Normal   | intermittent OpenCL regressiontest failures   |                | 03/02/2020 11:01 AM |                            |
| 3304 | GROMACS | Bug     | New                | Normal   | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5 | Michael Shirts | 03/01/2020 03:23 PM | 2020.2                     |
| 3294 | GROMACS | Bug     | New                | Normal   | multiple tests fail on fedora 31  | Paul Bauer     | 02/28/2020 03:12 PM | 2020.2                     |
| 3266 | GROMACS | Bug     | New                | High     | gmx density show wrong symmetrize density profile using -symm?                                  | Super duper    | 02/28/2020 08:24 AM | 2020.2                     |
| 3310 | GROMACS | Bug     | Blocked, need info | Low      | Thread affinity on Mac OS   |                | 02/27/2020 11:10 PM |                            |
| 3309 | GROMACS | Bug     | New                | Normal   | -reprod: checkpoint reading bug and general considerations                                      |                | 02/27/2020 10:45 PM |                            |
| 3050 | GROMACS | Bug     | New                | Low      | Fix tests on Solaris  | Vedran Miletic | 02/27/2020 11:05 AM | 2020.2                     |
| 3125 | GROMACS | Bug     | Resolved           | Normal   | OpenCL on Volta and Turing broken   |                | 02/27/2020 11:01 AM | 2020.2                     |
| 3249 | GROMACS | Bug     | In Progress        | Low      | cmake bad tests for avx512 on AMD   | Erik Lindahl   | 02/26/2020 05:00 PM |                            |
| 2974 | GROMACS | Bug     | New                | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                               |                | 02/25/2020 03:52 PM | 2020.2                     |
| 3071 | GROMACS | Bug     | Accepted           | Normal   | complex.nbnxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions               | Szilárd Páll   | 02/25/2020 03:39 PM | 2020.2                     |
| 3334 | GROMACS | Bug     | New                | Normal   | Check for DD when increasing rlist is broken  | Berk Hess      | 02/25/2020 03:28 PM | 2020.2                     |

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|------|---------|---------|--------------------|----------|--|---------------------|---------------------|----------------------------|
| 3398 | GROMACS | Bug     | New                | Normal   | Intermittent failure of non-bonded kernels when run using nvprof   |                     | 02/25/2020 12:14 PM |                            |
| 3333 | GROMACS | Bug     | New                | Normal   | Assertion failure when trying to get unit test help  | Paul Bauer          | 02/25/2020 10:16 AM | 2021-infrastructure-stable |
| 3387 | GROMACS | Bug     | New                | Normal   | Death test bug   |                     | 02/20/2020 05:39 PM |                            |
| 1166 | GROMACS | Bug     | New                | Low      | g_order is incorrect for unsaturated carbons   | David van der Spoel | 02/06/2020 02:32 PM | future                     |
| 3368 | GROMACS | Bug     | New                | Normal   | Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue | Vedat Durmaz        | 02/05/2020 04:51 PM | future                     |
| 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                       |
| 3305 | GROMACS | Bug     | New                | Normal   | Case gives FPE with Debug build when GPU update is enabled   |                     | 01/21/2020 05:44 PM |                            |
| 2733 | GROMACS | Bug     | Blocked, need info | Normal   | MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5  | Paul Bauer          | 01/17/2020 08:40 AM |                            |
| 3301 | GROMACS | Bug     | New                | Normal   | pdb2gmx adding hydrogen  |                     | 01/15/2020 10:17 PM |                            |
| 3240 | GROMACS | Bug     | New                | Normal   | segv with GPU DD direct communication with GPU update and -dlb off   |                     | 01/15/2020 06:16 PM |                            |
| 3265 | GROMACS | Bug     | Blocked, need info | Low      | regressiontests/complex fails on ppc64le   | Erik Lindahl        | 01/09/2020 05:00 PM |                            |
| 3284 | GROMACS | Bug     | New                | Normal   | gmx msd cannot output two xvg files as suggested by command line option  | Christian Blau      | 01/08/2020 04:50 PM | 2021-infrastructure-stable |
| 3281 | GROMACS | Bug     | New                | Normal   | Test data directory GMX_RELEASE_ASSERT triggers  |                     | 01/06/2020 08:07 PM |                            |
| 2832 | GROMACS | Bug     | New                | Low      | PaddedVector move operations broken  | Mark Abraham        | 12/28/2019 10:40 AM | 2021                       |
| 3274 | GROMACS | Bug     | New                | Normal   | Remove ARM NEON SIMD   |                     | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug     | New                | Normal   | gmxapi setup.py complains too much   |                     | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3101 | GROMACS | Bug     | Blocked, need info | Normal   | detect compilation failed  | Erik Lindahl        | 12/27/2019 10:52 AM |                            |
| 3075 | GROMACS | Bug     | New                | Normal   | Frozen atoms are moving  | Erik Lindahl        | 12/27/2019 10:51 AM |                            |
| 3210 | GROMACS | Bug     | New                | High     | rerun does not reproduce dVcoul/dl   |                     | 12/27/2019 10:45 AM |                            |
| 3244 | GROMACS | Bug     | In Progress        | Normal   | center of mass motion removal with position restraints can lead to artifacts                                       | Berk Hess           | 12/27/2019 10:40 AM | 2021                       |
| 3243 | GROMACS | Bug     | Feedback wanted    | Normal   | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning  |                     | 12/27/2019 10:31 AM |                            |
| 2987 | GROMACS | Bug     | New                | Normal   | assess the bonded GPU task assignment default  |                     | 12/20/2019 01:06 PM | 2021                       |
| 2480 | GROMACS | Bug     | New                | Normal   | pdb2gmx does not protonate correctly for united-atom Gromos  | Mark Abraham        | 12/20/2019 12:17 PM | 2021                       |
| 2390 | GROMACS | Bug     | Feedback wanted    | Normal   | GROMACS build system should check for valid nvcc flags before use  |                     | 12/20/2019 12:13 PM | 2021                       |
| 2192 | GROMACS | Bug     | Accepted           | Low      | grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error            | Berk Hess           | 12/20/2019 12:11 PM | 2021                       |

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| 1985 | GROMACS | Bug     | Fix uploaded | Low      | CUDA build system refactoring awaiting review   |                     | 12/20/2019 12:07 PM | 2021                       |
| 3246 | GROMACS | Bug     | Accepted     | Normal   | GPU code misses settle error check, simulation crashes with segfault without any further output   | Artem Zhmurov       | 12/20/2019 09:52 AM | 2021-infrastructure-stable |
| 3234 | GROMACS | Bug     | Accepted     | Normal   | Signal: Floating point exception Signal code: Floating point divide-by-zero   | Erik Lindahl        | 12/16/2019 03:40 PM |                            |
| 3239 | GROMACS | Bug     | New          | Normal   | GPU DD direct communication with GPU update error with RF   |                     | 12/14/2019 05:15 PM |                            |
| 3233 | GROMACS | Bug     | New          | Normal   | clang-format incorrectly aligning altered function arguments  |                     | 12/13/2019 12:41 PM |                            |
| 3136 | GROMACS | Bug     | New          | Normal   | gmxapi.operation data flow topology unclear or incomplete   | Eric Irrgang        | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 3141 | GROMACS | Bug     | New          | Normal   | gmxapi File placeholders missing from beta release  | Eric Irrgang        | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3228 | GROMACS | Bug     | New          | Normal   | gmxapi.commandline_operation should gracefully handle input/output file arguments   | Eric Irrgang        | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3227 | GROMACS | Bug     | New          | Normal   | solvate does not check return status of gmx_file_rename   |                     | 12/04/2019 01:43 PM |                            |
| 3223 | GROMACS | Bug     | New          | Normal   | unit test failures give verify -1   |                     | 12/02/2019 11:58 AM |                            |
| 3214 | GROMACS | Bug     | New          | Normal   | Out-of-bounds, overflow and incorrect outputs in gmx spatial  |                     | 11/25/2019 04:11 PM |                            |
| 3213 | GROMACS | Bug     | New          | Normal   | Having a local residuetypes.dat for custom force field  |                     | 11/21/2019 09:18 PM |                            |
| 3209 | GROMACS | Bug     | New          | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting   |                     | 11/19/2019 11:36 AM |                            |
| 3202 | GROMACS | Bug     | New          | Low      | gmx solvate fails to overwrite topology file  |                     | 11/13/2019 02:44 PM |                            |
| 3198 | GROMACS | Bug     | New          | Normal   | Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0 |                     | 11/06/2019 12:20 PM |                            |
| 3197 | GROMACS | Bug     | New          | Normal   | Rework usage of gitattributes and filter in source code formatting scripts  |                     | 11/04/2019 12:50 PM | 2021-infrastructure-stable |
| 3196 | GROMACS | Bug     | New          | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |                     | 11/01/2019 11:28 PM |                            |
| 3150 | GROMACS | Bug     | New          | Normal   | gmxapi data type annotations are confusing and inadequate   | Eric Irrgang        | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3166 | GROMACS | Bug     | New          | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1  |                     | 10/19/2019 09:13 PM |                            |
| 3165 | GROMACS | Bug     | New          | Normal   | task assignment silent abort  |                     | 10/18/2019 07:46 PM |                            |
| 3042 | GROMACS | Bug     | New          | Normal   | core dump error in grompp command   |                     | 10/09/2019 07:30 PM |                            |
| 3127 | GROMACS | Bug     | New          | Normal   | mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia  |                     | 10/09/2019 05:33 PM |                            |
| 3116 | GROMACS | Bug     | New          | Normal   | regressiontests/freeenergy core dumps on ppc64le  | Paul Bauer          | 10/04/2019 10:52 PM |                            |
| 3113 | GROMACS | Bug     | New          | Low      | Use of read_tps_conf is deprecated  | Paul Bauer          | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 3086 | GROMACS | Bug     | New          | Normal   | gmxapi fails with MPI build of GROMACS 2020   |                     | 09/25/2019 04:18 PM |                            |
| 3049 | GROMACS | Bug     | New          | Low      | gmx nmeig should plot a real infrared spectrum  | David van der Spoel | 09/24/2019 03:25 PM | future                     |
| 3088 | GROMACS | Bug     | New          | Normal   | Reference to theory needed for cylindrical pull geometry  |                     | 09/13/2019 11:26 AM |                            |

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|------|---------|---------|--------------------|----------|---|----------------|---------------------|----------------|
| 3083 | GROMACS | Bug     | New                | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build  |                | 09/10/2019 11:56 AM |                |
| 3058 | GROMACS | Bug     | Feedback wanted    | Normal   | Error when using a large PME grid on a GPU  |                | 09/04/2019 07:26 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 |                |
| 3068 | GROMACS | Bug     | New                | Normal   | Misleading warning on rerun   |                | 08/26/2019 03:44 PM |                |
| 3066 | GROMACS | Bug     | New                | Normal   | Gauss transform and density fit classes should operate on real values instead of float  | Christian Blau | 08/26/2019 11:53 AM |                |
| 3055 | GROMACS | Bug     | Feedback wanted    | Normal   | Error in gmx xpm2ps   |                | 08/22/2019 03:27 PM |                |
| 3054 | GROMACS | Bug     | New                | Normal   | Missing dihedral define   |                | 08/02/2019 05:47 PM |                |
| 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 |                |
| 2907 | GROMACS | Bug     | New                | Normal   | Gromacs autocompletion appears to be broken with ZSH  |                | 07/16/2019 04:46 AM |                |
| 3028 | GROMACS | Bug     | Feedback wanted    | Normal   | install fail on Centos 6  |                | 07/15/2019 12:32 PM |                |
| 2949 | GROMACS | Bug     | New                | Normal   | cmake fails when building mdrun only  |                | 07/08/2019 10:04 AM |                |
| 2762 | GROMACS | Bug     | Blocked, need info | Normal   | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads  |                | 07/01/2019 11:26 PM |                |
| 3000 | GROMACS | Bug     | New                | Normal   | CMake "webpage" target does not fail when it should   |                | 06/25/2019 02:43 PM |                |
| 2981 | GROMACS | Bug     | New                | Normal   | segfault in opencl build  |                | 06/18/2019 03:30 AM |                |
| 2980 | GROMACS | Bug     | New                | Normal   | taskassignment fails with unit tests when GPUs and custom number of ranks is used   |                | 06/17/2019 05:28 PM |                |
| 2734 | GROMACS | Bug     | In Progress        | Normal   | regressiontests/kernel core dumps on ppc64le  | Paul Bauer     | 06/15/2019 04:12 PM | future         |
| 2978 | GROMACS | Bug     | New                | Normal   | Some suggestions about the gmx current tool   |                | 06/13/2019 12:41 PM |                |
| 2954 | GROMACS | Bug     | New                | Normal   | genion changes residue numbering  |                | 05/26/2019 12:08 AM |                |
| 2948 | GROMACS | Bug     | New                | Normal   | SIMD support detected as none on AMD R5 2500U   |                | 05/21/2019 12:58 PM |                |
| 2902 | GROMACS | Bug     | New                | Normal   | 2019.1 equilibration issue? (Intel 2018u3)  |                | 04/30/2019 08:17 AM |                |
| 2924 | GROMACS | Bug     | New                | Normal   | Failing version check when reading new tpr file with older gromacs version  |                | 04/12/2019 10:52 AM |                |
| 2897 | GROMACS | Bug     | New                | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build   |                | 04/04/2019 06:24 PM |                |
| 2702 | GROMACS | Bug     | Accepted           | Normal   | PME gather reduction race in OpenCL (and CUDA)  |                | 03/28/2019 03:14 PM |                |
| 2876 | GROMACS | Bug     | New                | Normal   | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3)  | Erik Lindahl   | 03/08/2019 10:32 AM |                |
| 2883 | GROMACS | Bug     | New                | Normal   | essentialdynamics fail with Intel MPI   |                | 03/08/2019 03:10 AM |                |
| 2869 | GROMACS | Bug     | New                | Normal   | GPU detection error only issued as a note to the log  |                | 03/05/2019 04:09 PM |                |

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|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------|
| 2870 | GROMACS | Bug     | New             | Normal   | GPU detection error message missing from the output                                       |                     | 03/05/2019 03:55 PM |                |
| 2873 | GROMACS | Bug     | New             | Normal   | Simple way to get last frame from trajectory  |                     | 02/28/2019 11:14 PM |                |
| 2872 | GROMACS | Bug     | New             | Normal   | gmx solvate and genion topology update  |                     | 02/27/2019 10:18 AM |                |
| 2754 | GROMACS | Bug     | New             | Normal   | Simulated Tempering seems to be broken  | Michael Shirts      | 02/05/2019 03:58 PM |                |
| 2853 | GROMACS | Bug     | New             | Normal   | EwaldUnitTests segfault on armv7hl with gcc-9.0.1   | Paul Bauer          | 02/04/2019 05:34 PM |                |
| 2854 | GROMACS | Bug     | New             | Normal   | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1                                     | Paul Bauer          | 02/04/2019 11:17 AM |                |
| 2852 | GROMACS | Bug     | New             | Low      | the in-tree regressiontest download can get out of sync with code                         |                     | 01/30/2019 03:58 PM |                |
| 2848 | GROMACS | Bug     | New             | Normal   | gmx make_ndx ignores last residue in case only CA's are present in GRO file               |                     | 01/30/2019 06:16 AM |                |
| 2828 | GROMACS | Bug     | Feedback wanted | Normal   | Installation issue on Power 9 system with SIMD support                                    |                     | 01/18/2019 11:54 AM |                |
| 1354 | GROMACS | Bug     | New             | Normal   | Constant acceleration NEMD is broken.   | David van der Spoel | 01/09/2019 04:42 PM |                |
| 2788 | GROMACS | Bug     | New             | Normal   | PME will not run on AMD GPU with NVidia GPU present                                       |                     | 01/03/2019 02:24 PM |                |
| 2693 | GROMACS | Bug     | New             | Normal   | Several memory leaks in mdrun   |                     | 12/18/2018 04:22 AM | future         |
| 2649 | GROMACS | Bug     | New             | Normal   | Virial calculation necessary for correct energy calculation on GPU                        |                     | 12/17/2018 02:32 PM | future         |
| 2468 | GROMACS | Bug     | New             | Low      | incorrect GPU timing reported with OpenCL and domain decomposition                        |                     | 12/17/2018 01:28 PM | future         |
| 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 |                |
| 2065 | GROMACS | Bug     | New             | Normal   | thread-MPI internal errors  |                     | 11/08/2018 03:43 PM |                |
| 2740 | GROMACS | Bug     | New             | Normal   | mdrun reports incorrect error with -bonded gpu without gpu                                | Mark Abraham        | 11/07/2018 01:59 PM |                |
| 2707 | GROMACS | Bug     | New             | Normal   | Installed OpenCL files include clh file from gpu_utils directory                          |                     | 10/30/2018 04:02 AM |                |
| 2598 | GROMACS | Bug     | New             | Normal   | Tools using read_next_x cannot read TNG files with sanitizers                             |                     | 10/15/2018 01:16 PM | future         |
| 1919 | GROMACS | Bug     | Accepted        | Normal   | static linking issues cause by hwloc support  |                     | 10/12/2018 10:49 PM | future         |
| 2483 | GROMACS | Bug     | New             | Low      | gmx dump writes mdp files that can not be parsed by grompp                                | Paul Bauer          | 10/08/2018 10:50 AM | future         |
| 1880 | GROMACS | Bug     | Feedback wanted | Normal   | PP-PME load balancing issue   | Berk Hess           | 10/03/2018 09:45 PM | future         |
| 2645 | GROMACS | Bug     | New             | Normal   | Security  |                     | 09/28/2018 01:16 PM |                |
| 2657 | GROMACS | Bug     | New             | Normal   | Biphasic tutorial   |                     | 09/28/2018 10:02 AM |                |
| 2637 | GROMACS | Bug     | New             | High     | gmx solvate tears apart molecules   |                     | 09/11/2018 07:43 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 |                |
| 2624 | GROMACS | Bug     | New             | Normal   | GPU build system not robust enough  |                     | 09/05/2018 02:00 AM |                |

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| 2544 | GROMACS | Bug     | New                | Normal   | gmx rmsf does not fix periodicity in reference structure  | David van der Spoel | 08/21/2018 10:36 AM | future         |
| 2611 | GROMACS | Bug     | New                | Normal   | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX  |                     | 08/14/2018 07:03 PM |                |
| 2602 | GROMACS | Bug     | New                | Low      | build information gets outdated if build tree is reused   |                     | 08/13/2018 09:04 PM |                |
| 2607 | GROMACS | Bug     | New                | Normal   | Grompp becomes extremely slow when many pull groups are present   |                     | 08/11/2018 08:54 AM |                |
| 2606 | GROMACS | Bug     | New                | Normal   | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert                                    |                     | 08/10/2018 01:48 AM |                |
| 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 |                |
| 2576 | GROMACS | Bug     | New                | Normal   | gmx potential -correct outputs the wrong potential  |                     | 07/25/2018 02:58 PM |                |
| 2582 | GROMACS | Bug     | Blocked, need info | Normal   | Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6   | Szilárd Páll        | 07/23/2018 07:46 PM |                |
| 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 |                |
| 2568 | GROMACS | Bug     | New                | Low      | gmx editconf -rotate does not rotate the box  |                     | 07/10/2018 10:27 AM | future         |
| 2567 | GROMACS | Bug     | New                | Normal   | make check fails at test 23 SIMD errors   |                     | 07/10/2018 09:35 AM |                |
| 2564 | GROMACS | Bug     | New                | Normal   | Result Summary Different For Jobs With Different Numbers of Nodes   |                     | 07/05/2018 02:39 PM |                |
| 2555 | GROMACS | Bug     | New                | Low      | building GROMACS 2018.2   |                     | 07/03/2018 11:41 PM |                |
| 2563 | GROMACS | Bug     | New                | Normal   | Windows 7 Compilation with GPU support  |                     | 07/02/2018 09:58 AM |                |
| 2513 | GROMACS | Bug     | Feedback wanted    | Normal   | ref_t and temperature incorrect with coulomb-type = user  | Yu Du               | 05/31/2018 04:05 PM |                |
| 2526 | GROMACS | Bug     | New                | Normal   | Bug of gmx hbond  |                     | 05/30/2018 03:12 PM |                |
| 2482 | GROMACS | Bug     | Feedback wanted    | Normal   | Atoms/molecules in freezegrps move and system crashes   |                     | 05/18/2018 07:13 PM |                |
| 2473 | GROMACS | Bug     | New                | Normal   | mddrun sometimes stalls due to large coordinates with no constraints  |                     | 04/04/2018 10:15 PM |                |
| 2460 | GROMACS | Bug     | New                | Normal   | Allow inclusion of user libraries through CMake cache variables   |                     | 03/28/2018 08:47 PM |                |
| 2113 | GROMACS | Bug     | New                | Normal   | Google tests and execution order  |                     | 03/05/2018 02:05 PM |                |
| 2211 | GROMACS | Bug     | New                | Low      | gmx writes normal output to stderr  |                     | 03/05/2018 02:00 PM | future         |
| 2233 | GROMACS | Bug     | Accepted           | Normal   | replica exchange and -append bugged?  |                     | 03/05/2018 01:38 PM |                |
| 2427 | GROMACS | Bug     | New                | Normal   | gmx select gives syntax error for selection involving evaluating simple arithmetic expression                       |                     | 02/27/2018 05:15 PM |                |
| 2393 | GROMACS | Bug     | New                | Normal   | incorrect error message with omitted command line flag before its argument  |                     | 01/24/2018 11:24 PM |                |
| 2380 | GROMACS | Bug     | New                | Low      | cycle counter issues with separate PME rank + GPUs  |                     | 01/16/2018 10:21 PM |                |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee            | Updated             | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------|
| 2231 | GROMACS | Bug     | New             | Normal   | convert-tpr aborts when saving subset of the system   |                     | 01/12/2018 03:52 PM |                |
| 2052 | GROMACS | Bug     | New             | Low      | trjconv does not recognize periodic molecules   | David van der Spoel | 01/12/2018 11:05 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 |                |
| 1583 | GROMACS | Bug     | New             | Normal   | gmx msd with mol flag requires excessive memory   |                     | 12/18/2017 03:34 PM |                |
| 2255 | GROMACS | Bug     | New             | Normal   | nstlist override stopped affecting the input parameter listing  |                     | 12/17/2017 08:05 AM |                |
| 2252 | GROMACS | Bug     | New             | Low      | Memory allocation failures with large page sizes during PME tuning  |                     | 12/14/2017 04:27 AM |                |
| 2039 | GROMACS | Bug     | New             | Normal   | mdrun -pinstride defaults are too confusing   |                     | 12/13/2017 04:14 AM |                |
| 1811 | GROMACS | Bug     | New             | Normal   | Extrac build issues   |                     | 12/13/2017 03:43 AM |                |
| 2217 | GROMACS | Bug     | New             | Low      | GPU emulation and separate PME ranks doesn't work properly  |                     | 12/12/2017 11:50 AM |                |
| 1827 | GROMACS | Bug     | New             | Low      | cmake multi-configuration generator support partly broken   |                     | 12/11/2017 05:20 PM | future         |
| 2232 | GROMACS | Bug     | New             | Normal   | pdb2gmx can't form special bonds with terminal patched atoms  |                     | 12/03/2017 01:35 PM |                |
| 2241 | GROMACS | Bug     | New             | Low      | refdata can segfault when reading   |                     | 09/07/2017 11:57 AM |                |
| 2208 | GROMACS | Bug     | New             | Normal   | cuFFT linking   |                     | 06/30/2017 01:58 PM |                |
| 2147 | GROMACS | Bug     | Feedback wanted | Normal   | Parrinello-Rahman barostat not properly working   |                     | 06/06/2017 07:53 AM |                |
| 2020 | GROMACS | Bug     | New             | Normal   | Possible issue with md-vv integrator  | Mark Abraham        | 03/11/2017 08:30 AM |                |
| 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 |                |
| 1843 | GROMACS | Bug     | In Progress     | Normal   | pbcs=xy with 2 walls floating point exception with the verlet scheme  | Berk Hess           | 10/31/2016 11:35 AM |                |
| 1442 | GROMACS | Bug     | Feedback wanted | Normal   | Not consistent solvation free energies differencies   | Michael Shirts      | 07/11/2016 08:13 PM |                |
| 1934 | GROMACS | Bug     | New             | Normal   | QMMM with ORCA: memory leaks, buffer overflows and much more  |                     | 07/10/2016 09:26 AM |                |
| 1839 | GROMACS | Bug     | Accepted        | Low      | pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx   |                     | 07/09/2016 07:27 PM | future         |
| 1667 | GROMACS | Bug     | New             | Normal   | gmx convert-tpr writes wrong number of mol in output tpr  | David van der Spoel | 06/27/2016 08:29 PM |                |
| 1448 | GROMACS | Bug     | New             | Normal   | multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing) | Mark Abraham        | 06/23/2016 03:15 PM |                |
| 1568 | GROMACS | Bug     | New             | Low      | inconsistent/incorrect threading checks and reporting in mdrun  |                     | 05/25/2016 02:01 AM |                |
| 1476 | GROMACS | Bug     | New             | Low      | Odd behavior with verlet-buffer-drift   |                     | 05/25/2016 01:45 AM | future         |
| 1618 | GROMACS | Bug     | In Progress     | Normal   | g_protonate segfaults unconditionally   | Erik Lindahl        | 08/17/2015 02:10 PM |                |

| #    | Project                | Tracker | Status          | Priority | Subject   | Assignee            | Updated             | Target version             |
|------|------------------------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 1770 | GROMACS                | Bug     | New             | Normal   | segmentation fault with free energy changes and multiple GPU's  |                     | 07/14/2015 03:24 AM |                            |
| 1648 | GROMACS                | Bug     | Feedback wanted | Normal   | Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges | Michael Shirts      | 06/25/2015 06:07 AM |                            |
| 1235 | GROMACS                | Bug     | New             | Normal   | peptide dihedral angle definitions violate IUPAC  | David van der Spoel | 06/19/2015 12:24 AM | future                     |
| 1339 | GROMACS                | Bug     | New             | Normal   | Center of mass drift with Nose-Hoover, MTK and md-vv  | Michael Shirts      | 06/18/2015 08:53 PM | future                     |
| 1730 | GROMACS                | Bug     | New             | Normal   | gmx compare does not compare all fields of a .tpr   |                     | 06/12/2015 09:33 PM | future                     |
| 1655 | GROMACS                | Bug     | New             | Normal   | g_membed and box type   |                     | 12/09/2014 01:33 PM |                            |
| 1190 | GROMACS                | Bug     | New             | Normal   | Use of FORCE in setting cached variables  | Mark Abraham        | 06/17/2014 06:09 AM |                            |
| 1481 | GROMACS                | Bug     | New             | Low      | g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files                    | David van der Spoel | 06/12/2014 01:37 PM |                            |
| 2935 | Support Platforms      | Bug     | New             | High     | redmine issue updates about gerrit uploads stopped working  |                     | 06/11/2019 01:42 PM | current                    |
| 1836 | Support Platforms      | Bug     | New             | Normal   | Support a way to retrigger part of matrix job   |                     | 07/22/2017 12:30 AM |                            |
| 2096 | Support Platforms      | Bug     | New             | Normal   | Redmine internal error with special characters  |                     | 05/31/2017 08:48 PM |                            |
| 1731 | Support Platforms      | Bug     | In Progress     | Normal   | document jenkins configuration and set up means to track changes  |                     | 05/31/2017 06:13 PM |                            |
| 1551 | Support Platforms      | Bug     | Feedback wanted | Normal   | git index.lock issue  |                     | 05/31/2017 05:37 PM |                            |
| 2149 | Support Platforms      | Bug     | New             | Normal   | gerrit server excessive CPU usage   |                     | 04/05/2017 07:25 PM |                            |
| 1967 | Support Platforms      | Bug     | Resolved        | Normal   | Documentation pages generated by Jenkins do not render properly   |                     | 08/27/2016 02:04 AM |                            |
| 1732 | Support Platforms      | Bug     | New             | Normal   | review and extend jenkins tests setups, coverage  |                     | 05/03/2016 05:30 AM |                            |
| 2937 | TNG trajectory library | Bug     | New             | Normal   | tng_num_frames_get reports incorrect num frames   |                     | 04/29/2019 11:30 AM |                            |
| 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 |                            |
| 1536 | TNG trajectory library | Bug     | New             | Normal   | TNG uses incorrect format for size_t on 32bit   |                     | 06/28/2014 03:56 AM |                            |
| 1252 | TNG trajectory library | Bug     | Feedback wanted | Normal   | residual ids and atomIDs  | Magnus Lundborg     | 06/12/2013 10:35 AM | version 1                  |
| 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 |                            |
| 2254 | GROMACS                | Feature | Resolved        | Normal   | GPU extensions for Google Tests   |                     | 10/06/2020 12:15 PM |                            |
| 3417 | GROMACS                | Feature | New             | Normal   | Make modular simulator feature-complete   | Pascal Merz         | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3311 | GROMACS                | Feature | In Progress     | Normal   | GPU infrastructure development  |                     | 03/20/2020 09:54 AM | 2021-refactoring           |
| 3395 | GROMACS                | Feature | Feedback wanted | Normal   | Consider scripted composition of Dockerfiles  |                     | 03/16/2020 12:16 PM |                            |



| #    | Project | Tracker | Status          | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|---------------------|---------------------|----------------------------|
| 3426 | GROMACS | Feature | New             | Normal   | Support acceleration in modular simulator  | Pascal Merz         | 03/11/2020 04:09 PM | 2021-infrastructure-stable |
| 3439 | GROMACS | Feature | New             | Normal   | Optimize successive simulation segments  |                     | 03/11/2020 01:42 PM |                            |
| 3433 | GROMACS | Feature | New             | Normal   | Decide how to handle multisim with modular simulator                                   | Pascal Merz         | 03/11/2020 06:42 AM | 2021-infrastructure-stable |
| 3436 | GROMACS | Feature | New             | Normal   | Implement AWH for modular simulator  | Pascal Merz         | 03/11/2020 06:32 AM | 2021-infrastructure-stable |
| 3435 | GROMACS | Feature | New             | Normal   | Implement pull for modular simulator   | Pascal Merz         | 03/11/2020 06:31 AM | 2021-infrastructure-stable |
| 3434 | GROMACS | Feature | New             | Normal   | Support box deformation in modular simulator   | Pascal Merz         | 03/11/2020 12:50 AM | 2021-infrastructure-stable |
| 3432 | GROMACS | Feature | New             | Normal   | Implement essential dynamics for modular simulator                                     | Pascal Merz         | 03/11/2020 12:38 AM | 2021-infrastructure-stable |
| 3431 | GROMACS | Feature | New             | Normal   | Implement virtual sites for modular simulator  | Pascal Merz         | 03/11/2020 12:33 AM | 2021-infrastructure-stable |
| 3430 | GROMACS | Feature | New             | Normal   | Implement NMR restraints for modular simulator   | Pascal Merz         | 03/11/2020 12:28 AM | 2021-infrastructure-stable |
| 3428 | GROMACS | Feature | New             | Normal   | Implement SIMD version of modular simulator propagators                                | Pascal Merz         | 03/11/2020 12:12 AM | 2021-infrastructure-stable |
| 3427 | GROMACS | Feature | New             | Normal   | Support freeze groups in modular simulator   | Pascal Merz         | 03/11/2020 12:07 AM | 2021-infrastructure-stable |
| 3425 | GROMACS | Feature | New             | Normal   | Implement rerun for the modular simulator  | Pascal Merz         | 03/10/2020 11:57 PM | 2021-infrastructure-stable |
| 3424 | GROMACS | Feature | New             | Normal   | Implement stochastic dynamics / langevin integrator in modular simulator               | Pascal Merz         | 03/10/2020 11:48 PM | 2021-infrastructure-stable |
| 3423 | GROMACS | Feature | New             | Normal   | Implement additional temperature and pressure control algorithms for modular simulator | Pascal Merz         | 03/10/2020 11:22 PM | 2021-infrastructure-stable |
| 3410 | GROMACS | Feature | New             | Normal   | Random Acceleration Molecular Dynamics (RAMD)  | Bernd Doser         | 03/05/2020 03:22 PM | 2021                       |
| 3374 | GROMACS | Feature | New             | Normal   | SimulationInput abstraction  |                     | 03/03/2020 05:32 PM | 2021-refactoring           |
| 3021 | GROMACS | Feature | Feedback wanted | Normal   | Completion of docs for GPU developments  |                     | 03/02/2020 03:58 PM | 2020.2                     |
| 3363 | GROMACS | Feature | New             | Normal   | Improve FEP testing  | Pascal Merz         | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3242 | GROMACS | Feature | New             | Normal   | Please do not remove the -nsteps flag  |                     | 03/01/2020 01:59 PM |                            |
| 3298 | GROMACS | Feature | New             | Normal   | start early PP work for first dimension of halo exchange                               |                     | 03/01/2020 01:36 PM |                            |
| 2667 | GROMACS | Feature | New             | Normal   | Suggested steps for calculating entropy in solution and binding                        | David van der Spoel | 03/01/2020 01:35 PM | 2020.2                     |
| 3283 | GROMACS | Feature | Resolved        | Normal   | Support for the string method with swarms of trajectories in GROMACS                   |                     | 03/01/2020 01:16 PM | 2021                       |
| 3379 | GROMACS | Feature | New             | Normal   | C++ API for simulation input and output  |                     | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3285 | GROMACS | Feature | Resolved        | Normal   | Run simulations from the same tpr file with different random seeds                     |                     | 02/27/2020 11:22 PM | future                     |
| 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 |
| 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 |
| 3393 | GROMACS | Feature | Resolved        | Normal   | Allow gmxapi.commandline_operation to use STDIN  | Eric Irrgang        | 02/25/2020 05:15 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee         | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|------------------|---------------------|----------------------------|
| 3394 | GROMACS | Feature | New             | Normal   | improve gmxapi error handling   | Eric Irrgang     | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3117 | GROMACS | Feature | New             | Normal   | Coulomb FEP PME on GPU  | Magnus Lundborg  | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 2915 | GROMACS | Feature | In Progress     | High     | GPU direct communications   |                  | 02/14/2020 12:48 PM |                            |
| 2890 | GROMACS | Feature | In Progress     | Normal   | GPU Halo Exchange   |                  | 02/14/2020 12:41 PM | 2021                       |
| 2891 | GROMACS | Feature | In Progress     | Normal   | PME/PP GPU communications   |                  | 02/14/2020 12:40 PM |                            |
| 3160 | GROMACS | Feature | Fix uploaded    | High     | implement direct comm for different src/target memory spaces          | Alan Gray        | 02/14/2020 11:28 AM | 2021-infrastructure-stable |
| 3378 | GROMACS | Feature | New             | Normal   | genion usage without stdin (facilitates use in gmx python api)        |                  | 02/13/2020 12:04 PM |                            |
| 3355 | GROMACS | Feature | Accepted        | Normal   | New PME parallel (GPU) scheme   | Jonathan Vincent | 02/12/2020 11:58 AM |                            |
| 3114 | GROMACS | Feature | New             | Normal   | Improve GPU update-constraints module                                 | Artem Zhmurov    | 02/10/2020 04:30 PM | 2021                       |
| 2601 | GROMACS | Feature | New             | Normal   | Free energy calculations, soft-core potential                         | Vytautas Gapsys  | 02/10/2020 11:29 AM | future                     |
| 3371 | GROMACS | Feature | New             | Normal   | Control FEP using AWH   | Magnus Lundborg  | 02/06/2020 02:20 PM | 2021                       |
| 3369 | GROMACS | Feature | New             | Normal   | Add quote about "the truth"   |                  | 02/05/2020 05:08 PM |                            |
| 3362 | GROMACS | Feature | New             | Normal   | gmx traj: add an option to plot each component in a separate file     |                  | 01/29/2020 06:18 PM |                            |
| 2967 | GROMACS | Feature | New             | Normal   | GPU reallocateDeviceBuffer improvements                               |                  | 01/23/2020 12:15 PM | 2021-refactoring           |
| 3318 | GROMACS | Feature | In Progress     | Normal   | Use wrappers for the GPU buffer copy/allocations                      | Artem Zhmurov    | 01/23/2020 12:01 PM | 2021-refactoring           |
| 3313 | GROMACS | Feature | Accepted        | Normal   | Introduce and use opaque types for the DeviceStream and DeviceContext | Artem Zhmurov    | 01/23/2020 12:00 PM | 2021-refactoring           |
| 3352 | GROMACS | Feature | New             | Normal   | GPU update-constraints feature support                                | Artem Zhmurov    | 01/23/2020 11:59 AM | 2021                       |
| 3351 | GROMACS | Feature | New             | Normal   | GPU update-constraints code organization and integration              | Artem Zhmurov    | 01/23/2020 11:59 AM | 2021                       |
| 3350 | GROMACS | Feature | New             | Normal   | GPU update-constraints performance                                    | Artem Zhmurov    | 01/23/2020 11:59 AM | 2021                       |
| 3307 | GROMACS | Feature | New             | Normal   | General interface for communication between simulation ranks          |                  | 01/22/2020 03:22 PM | 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 |                            |
| 3328 | GROMACS | Feature | New             | Normal   | Testing framework for task assignment                                 |                  | 01/22/2020 09:48 AM | 2021-refactoring           |
| 3172 | GROMACS | Feature | New             | Normal   | QM/MM Interface with CP2K   | Dmitry Morozov   | 01/17/2020 12:18 PM | future                     |
| 2896 | GROMACS | Feature | Feedback wanted | Normal   | Python packaging  |                  | 01/16/2020 07:11 PM | 2021-refactoring           |
| 3295 | GROMACS | Feature | New             | Normal   | Expand gmxapi.modify_input use cases.                                 | Eric Irrgang     | 01/16/2020 05:13 PM | 2021-refactoring           |
| 3152 | GROMACS | Feature | New             | Normal   | Infrastructure and patterns for expressing public interfaces          |                  | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 1347 | GROMACS | Feature | New             | Normal   | future of tables  | Berk Hess        | 01/09/2020 02:37 PM | future                     |
| 2070 | GROMACS | Feature | In Progress     | Normal   | Physical validation testing   | Michael Shirts   | 01/03/2020 09:36 PM | future                     |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee            | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 3277 | GROMACS | Feature | New             | Normal   | Allow testing feature that is partly implemented                              |                     | 12/31/2019 12:44 PM | 2021                       |
| 2710 | GROMACS | Feature | New             | Normal   | Separate dvl for each molecule (of couple-moltype) when running FEP           |                     | 12/27/2019 04:41 PM | 2021                       |
| 2715 | GROMACS | Feature | New             | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support       |                     | 12/27/2019 04:06 PM | future                     |
| 2774 | GROMACS | Feature | New             | Normal   | Refactor shell code into its own integrator                                   | David van der Spoel | 12/27/2019 04:05 PM | 2021                       |
| 2944 | GROMACS | Feature | New             | Normal   | Roadmap for thermostats / barostats in new propagation/integration scheme     | Michael Shirts      | 12/27/2019 04:00 PM | 2021                       |
| 2806 | GROMACS | Feature | New             | Normal   | SIMD algorithms for ARM SVE // nobnonded cluster and others                   |                     | 12/27/2019 03:59 PM | 2021                       |
| 2581 | GROMACS | Feature | Accepted        | Normal   | User interface for hybrid Monte Carlo   |                     | 12/20/2019 12:24 PM | future                     |
| 2054 | GROMACS | Feature | Accepted        | High     | PME on GPU  | Aleksei lupinov     | 12/20/2019 12:18 PM | future                     |
| 2224 | GROMACS | Feature | New             | Normal   | Proposed feature: conditional stop  | Vedran Miletic      | 12/20/2019 12:11 PM | 2021                       |
| 1165 | GROMACS | Feature | Accepted        | Low      | Multi-SIMD binaries   |                     | 12/20/2019 12:00 PM | future                     |
| 868  | GROMACS | Feature | In Progress     | Normal   | Implement parallelization support to analysis framework                       | Kevin Boyd          | 12/20/2019 11:59 AM | 2021                       |
| 2585 | GROMACS | Feature | Resolved        | Normal   | Infrastructure supporting external API  |                     | 12/11/2019 12:39 PM |                            |
| 2994 | GROMACS | Feature | New             | Normal   | Data flow topology in gmxapi 2020   |                     | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 3032 | GROMACS | Feature | Feedback wanted | Normal   | Clean up dev-manual structure   |                     | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3140 | GROMACS | Feature | New             | Normal   | Allow explicit input definition for gmxapi.operation function wrapper         | Eric Irrgang        | 12/10/2019 02:00 PM | 2021-infrastructure-stable |
| 3038 | GROMACS | Feature | New             | Normal   | Improvements to MD plugin development environment                             | Eric Irrgang        | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 2996 | GROMACS | Feature | In Progress     | Normal   | gmxapi execution model  | Eric Irrgang        | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 2961 | GROMACS | Feature | New             | Normal   | How should Python package find GROMACS resources under various circumstances? |                     | 12/09/2019 10:47 AM |                            |
| 3177 | GROMACS | Feature | New             | Normal   | Spack package management support  |                     | 11/06/2019 06:37 PM |                            |
| 2126 | GROMACS | Feature | New             | Normal   | implement native CUDA support in CMake  |                     | 10/29/2019 09:03 PM |                            |
| 3179 | GROMACS | Feature | New             | Normal   | Clarify access to parallel data outputs                                       | Eric Irrgang        | 10/26/2019 12:23 PM |                            |
| 2993 | GROMACS | Feature | New             | Normal   | Scalar and structured type expression and definitions for API                 | Eric Irrgang        | 10/17/2019 09:55 AM |                            |
| 3148 | GROMACS | Feature | New             | Normal   | Roadmap for gmxapi filesystem interactions.                                   | Eric Irrgang        | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3149 | GROMACS | Feature | New             | Normal   | Python user interface for obtaining simulation artifacts as files.            | Eric Irrgang        | 10/15/2019 06:21 PM |                            |
| 3147 | GROMACS | Feature | New             | Normal   | gmxapi workflow checkpointing   | Eric Irrgang        | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3138 | GROMACS | Feature | New             | Normal   | Improve ensemble support in Context specification.                            |                     | 10/15/2019 03:56 PM |                            |
| 3135 | GROMACS | Feature | New             | Normal   | Make GPU traits into opaque types   |                     | 10/14/2019 10:24 AM |                            |
| 3134 | GROMACS | Feature | Feedback wanted | Normal   | gmxapi Python exception names may need improvement                            | Eric Irrgang        | 10/13/2019 01:50 PM |                            |

| #    | 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 |                |
| 3115 | GROMACS | Feature | New         | Normal   | Device stream manager   |                     | 10/04/2019 09:00 AM |                |
| 2451 | GROMACS | Feature | Resolved    | Normal   | Linear virtual sites with fixed distance                                    | David van der Spoel | 09/16/2019 01:15 PM |                |
| 3069 | GROMACS | Feature | New         | Low      | Iterator over span and indices into this span (zip-style iterator)          | Christian Blau      | 08/29/2019 11:11 AM | future         |
| 742  | GROMACS | Feature | New         | Normal   | Enhancing the performance of the free energy code                           |                     | 08/26/2019 04:55 PM | future         |
| 1500 | GROMACS | Feature | New         | Normal   | Post-5.0 feature clean-up plan  | Mark Abraham        | 08/26/2019 03:47 PM |                |
| 1665 | GROMACS | Feature | New         | Normal   | improve free energy non-bonded kernel performance                           |                     | 08/26/2019 03:47 PM | future         |
| 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 |                |
| 3030 | GROMACS | Feature | New         | Normal   | RST style guidelines  |                     | 07/09/2019 03:38 PM |                |
| 2034 | GROMACS | Feature | New         | Normal   | Unit tests for bonded forces  | David van der Spoel | 06/29/2019 10:22 AM | future         |
| 2984 | GROMACS | Feature | New         | Normal   | More Extensive Selections Examples  | Dallas Warren       | 06/18/2019 11:50 PM |                |
| 2977 | GROMACS | Feature | New         | Normal   | print DD load balancing improvement   |                     | 06/13/2019 10:56 AM |                |
| 2975 | GROMACS | Feature | New         | Normal   | LJ PME calculations on GPUs   |                     | 06/12/2019 01:17 PM |                |
| 2956 | GROMACS | Feature | New         | Normal   | SAXS resolution   |                     | 05/17/2019 09:58 AM |                |
| 2596 | GROMACS | Feature | New         | Normal   | Constant potential method   | Benson Muite        | 05/10/2019 09:54 AM |                |
| 2570 | GROMACS | Feature | New         | Normal   | Better string formatting and printing                                       |                     | 05/02/2019 12:20 PM |                |
| 2931 | GROMACS | Feature | New         | Normal   | Tables in Verlet kernels  |                     | 04/29/2019 12:01 PM |                |
| 2930 | GROMACS | Feature | New         | Normal   | Limited range for reference group detection in cylinder pulling             |                     | 04/26/2019 05:17 PM |                |
| 2928 | GROMACS | Feature | New         | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements. |                     | 04/16/2019 04:52 PM |                |
| 2910 | GROMACS | Feature | New         | Normal   | Mixed scaling for 1-4 interactions  |                     | 04/10/2019 10:13 PM |                |
| 2574 | GROMACS | Feature | New         | Normal   | iForceSchedule Abstraction  | Prashanth Kanduri   | 03/29/2019 05:20 PM | future         |
| 2282 | GROMACS | Feature | New         | Normal   | Density map toolset   | Christian Blau      | 03/21/2019 06:08 PM | future         |
| 2866 | GROMACS | Feature | New         | Normal   | Alternative non-bonded potentials   | David van der Spoel | 03/05/2019 03:50 PM | future         |
| 1625 | GROMACS | Feature | New         | Normal   | Gromacs Python API  |                     | 03/02/2019 01:44 AM | future         |
| 2068 | GROMACS | Feature | New         | Normal   | Access to low level classes   |                     | 03/02/2019 01:37 AM | future         |
| 2791 | GROMACS | Feature | In Progress | Normal   | Implement a module for lambda-dynamics simulations (lambda_site module)     | Thomas Ullmann      | 03/01/2019 01:36 AM | future         |
| 2111 | GROMACS | Feature | In Progress | Normal   | Implement Gaussian screening of electrostatics                              |                     | 02/23/2019 12:33 PM |                |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee            | Updated             | Target version |
|------|---------|---------|-------------|----------|---|---------------------|---------------------|----------------|
| 2594 | GROMACS | Feature | New         | Normal   | Multi-level GMX API   | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2755 | GROMACS | Feature | New         | Low      | md5 sums and sha256, sha512 hashes  | Benson Muite        | 02/19/2019 11:00 PM |                |
| 2860 | GROMACS | Feature | New         | Normal   | Option for outputting min/max coordinates in gmx traj   |                     | 02/08/2019 12:35 AM |                |
| 2248 | GROMACS | Feature | New         | Normal   | Label all SIMD functions as pure/nodiscard  |                     | 02/04/2019 04:49 AM |                |
| 2846 | GROMACS | Feature | New         | Low      | Set rpath in FindLibStdCpp.cmake  |                     | 02/02/2019 08:09 AM |                |
| 2840 | GROMACS | Feature | New         | Normal   | Test that functionality does not compile that is not supposed to.                                 |                     | 01/25/2019 02:35 PM | future         |
| 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         |
| 2239 | GROMACS | Feature | New         | Normal   | split libgromacs into base and full   |                     | 01/07/2019 01:47 AM |                |
| 2186 | GROMACS | Feature | New         | Low      | Potential change for logical improvements: move control of constraints purely to the .mdp         | Michael Shirts      | 11/27/2018 11:27 AM | future         |
| 2761 | GROMACS | Feature | New         | Low      | lincs-order 4 is too conservative for some force fields   |                     | 11/16/2018 09:55 AM |                |
| 2739 | GROMACS | Feature | New         | Normal   | Parallel continuous tempering and enhanced sampling feature                                       |                     | 11/13/2018 11:36 PM |                |
| 2713 | GROMACS | Feature | New         | Normal   | Constant offset for external electric fields  |                     | 10/28/2018 12:57 AM |                |
| 1168 | GROMACS | Feature | In Progress | Low      | g_density does not do what users think it does, given PBC over z and constant pressure simulation | Erik Lindahl        | 10/20/2018 12:49 AM | future         |
| 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 |                |
| 1666 | GROMACS | Feature | New         | Normal   | new approach for Verlet-scheme kernel generation  | Erik Lindahl        | 10/08/2018 07:04 PM | future         |
| 1511 | GROMACS | Feature | Accepted    | Normal   | add PDBx (ie mmCIF) support   |                     | 10/05/2018 07:14 PM |                |
| 2545 | GROMACS | Feature | New         | Normal   | Should grompp fix periodicity of input files?   | David van der Spoel | 10/03/2018 11:32 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         |
| 2310 | GROMACS | Feature | Accepted    | Low      | Let mdrun dump coordinates with non-finite energy   |                     | 10/03/2018 09:47 PM | future         |
| 2354 | GROMACS | Feature | New         | Normal   | develop configuration file support for control of task layout                                     |                     | 09/19/2018 03:01 PM | future         |
| 2643 | GROMACS | Feature | New         | Low      | mdp options and/or docs for anisotropic aspects of implementations                                |                     | 09/12/2018 02:23 PM |                |
| 2622 | GROMACS | Feature | New         | Low      | Reduce severity of Berendsen warning  |                     | 08/23/2018 11:16 PM | future         |
| 1972 | GROMACS | Feature | New         | Normal   | external potential modules for refinement against experimental data                               |                     | 08/22/2018 05:03 PM | future         |
| 2229 | GROMACS | Feature | New         | High     | Full Object Oriented Modularization of GROMACS MDRUN Codebase                                     | Mark Abraham        | 08/22/2018 05:03 PM | future         |
| 2579 | GROMACS | Feature | New         | Normal   | Add dimensionality option to gmx trjconv -center  |                     | 07/19/2018 04:53 PM | future         |
| 2556 | GROMACS | Feature | New         | Normal   | make default selections suitable for DNA and RNA  | Mark Abraham        | 06/20/2018 01:48 PM |                |

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee       | Updated             | Target version |
|------|---------|---------|-----------------|----------|---|----------------|---------------------|----------------|
| 2547 | GROMACS | Feature | New             | Low      | Add option of averaging and obtaining error bars for AWH PMFs                         | Viveca Lindahl | 06/06/2018 11:31 AM | future         |
| 2491 | GROMACS | Feature | New             | Low      | Allow constant bias AWH simulations   | Viveca Lindahl | 06/05/2018 10:38 PM | future         |
| 1332 | GROMACS | Feature | In Progress     | Normal   | Supporting multiple end states instead of just A and B                                | Michael Shirts | 06/05/2018 03:58 PM |                |
| 1652 | GROMACS | Feature | New             | Normal   | Decide how to represent multiple lambda states internally                             | Michael Shirts | 06/05/2018 03:58 PM |                |
| 1653 | GROMACS | Feature | New             | Normal   | Decide how to represent multiple lambda states in the .top file and how to parse them | Michael Shirts | 06/05/2018 03:58 PM |                |
| 2429 | GROMACS | Feature | New             | Normal   | Add option of periodic chain topology to pdb2gmx                                      |                | 03/10/2018 01:01 PM |                |
| 2428 | GROMACS | Feature | New             | Normal   | Add way of selecting interactive arguments of pdb2gmx by string rather than an index  |                | 02/27/2018 06:28 PM |                |
| 2005 | GROMACS | Feature | New             | Normal   | Full Correlation Analysis (FCA) as Trajectory Analysis Module                         | Christian Blau | 02/07/2018 02:19 PM | future         |
| 1842 | GROMACS | Feature | New             | Normal   | Replace XML with JSON   |                | 01/18/2018 05:12 PM |                |
| 2139 | GROMACS | Feature | New             | Normal   | More precise/explicit documentation conventions                                       |                | 01/07/2018 11:54 PM |                |
| 2288 | GROMACS | Feature | Accepted        | Low      | gmx msd doesn't optimally handle missing input trajectory frames                      |                | 11/10/2017 11:03 AM |                |
| 2289 | GROMACS | Feature | New             | Normal   | gmx spatial add ability to perform over multiple reference structures                 |                | 11/08/2017 12:31 AM |                |
| 2283 | GROMACS | Feature | New             | Normal   | Force distribution analysis   | Bernd Doser    | 10/27/2017 11:44 AM |                |
| 2218 | GROMACS | Feature | Feedback wanted | Normal   | A tiny feature: damping for umbrella pull   |                | 08/16/2017 07:20 PM |                |
| 2226 | GROMACS | Feature | New             | Normal   | Harmonise commands for exit in make_ndx and distance                                  |                | 08/04/2017 12:24 PM |                |
| 2220 | GROMACS | Feature | New             | Normal   | report relevant env var behaviour to console  |                | 07/31/2017 09:40 PM |                |
| 2207 | GROMACS | Feature | New             | Normal   | solvent excluded volume of large molecule with periodic boundary condition            |                | 06/16/2017 10:37 AM |                |
| 1948 | GROMACS | Feature | New             | Low      | add warning when non-identical GPUs are used  |                | 06/12/2017 08:45 PM |                |
| 2194 | GROMACS | Feature | Accepted        | Low      | xvg output requested as an output option in place of xpm files                        |                | 05/31/2017 04:26 PM |                |
| 1854 | GROMACS | Feature | New             | Normal   | Remove all cyclic dependencies  |                | 05/25/2017 08:34 AM |                |
| 2137 | GROMACS | Feature | New             | Normal   | Preliminary refactoring of constraints and update machinery.                          | Michael Shirts | 03/11/2017 08:32 AM | future         |
| 2132 | GROMACS | Feature | New             | Normal   | Intermediate code for xvg handling  |                | 03/08/2017 05:12 PM | future         |
| 1137 | GROMACS | Feature | New             | Normal   | Proposal for integrator framework (do_md) in future GROMACS                           | Michael Shirts | 02/21/2017 12:48 AM | future         |
| 2118 | GROMACS | Feature | New             | Low      | More verbose comments requested in header of gmx distance -xyz                        |                | 02/08/2017 05:46 AM |                |
| 2101 | GROMACS | Feature | New             | Low      | warnip could print the offending line, as well as its number                          |                | 01/20/2017 03:06 PM |                |
| 2097 | GROMACS | Feature | New             | Low      | Move output of dhd file entirely to edr, rather than having a separate text dhd file  |                | 01/05/2017 05:21 PM | future         |
| 2090 | GROMACS | Feature | New             | Normal   | redirecting stdout or stderr for testing  | Mark Abraham   | 12/15/2016 03:15 AM |                |
| 2080 | GROMACS | Feature | New             | Normal   | add grompp warning for suitability for domain decomposition                           |                | 11/23/2016 03:03 PM |                |

| #    | Project | Tracker | Status             | Priority | Subject  | Assignee               | Updated             | Target version |
|------|---------|---------|--------------------|----------|--|------------------------|---------------------|----------------|
| 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 |                |
| 720  | GROMACS | Feature | Accepted           | Low      | permit pdb2gmx to choose a kind of HIS based on proton position  |                        | 11/17/2016 03:51 PM | future         |
| 2060 | GROMACS | Feature | New                | Normal   | Convert enum to enum class   |                        | 10/17/2016 05:27 PM |                |
| 2056 | GROMACS | Feature | New                | Low      | rename "gmx select"  |                        | 10/03/2016 08:24 PM |                |
| 1715 | GROMACS | Feature | New                | Low      | improve cycle counting GPU sharing and multi-sim   |                        | 08/03/2016 12:32 PM | future         |
| 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 |                |
| 1994 | GROMACS | Feature | New                | Low      | explore using JIT for CUDA   |                        | 07/11/2016 10:20 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 |                |
| 1030 | GROMACS | Feature | Fix uploaded       | Low      | adding -tu option to some analysis tools   | Rossen Apostolov       | 07/11/2016 08:22 PM |                |
| 1083 | GROMACS | Feature | In Progress        | Normal   | Improve collective error/warning/note handling in mdrun  |                        | 07/11/2016 08:21 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 |                |
| 1192 | GROMACS | Feature | Accepted           | Normal   | Add support for Verlet scheme with Buckingham  | Berk Hess              | 07/11/2016 08:19 PM |                |
| 1303 | GROMACS | Feature | New                | Normal   | Adding lambda dependent distance for pull code   | Michael Shirts         | 07/11/2016 08:18 PM |                |
| 1328 | GROMACS | Feature | Accepted           | Normal   | Names for selection positions  |                        | 07/11/2016 08:15 PM |                |
| 1498 | GROMACS | Feature | New                | Low      | g_dipoles does not work properly with ionic systems  | David van der Spoel    | 07/11/2016 08:11 PM |                |
| 1562 | GROMACS | Feature | New                | Normal   | introducing a Monte Carlo framework (first application: MC barostat)   | Michael Shirts         | 07/11/2016 08:08 PM |                |
| 1627 | GROMACS | Feature | In Progress        | Normal   | DPD integrator   |                        | 07/11/2016 08:08 PM |                |
| 1654 | GROMACS | Feature | New                | Normal   | How to carry out movement between chemical end states in a multiple end state framework?   | Michael Shirts         | 07/11/2016 08:05 PM |                |
| 1658 | GROMACS | Feature | New                | Normal   | Electrostatics treatment for multiple lambda sites   | Berk Hess              | 07/11/2016 08:05 PM |                |
| 1849 | GROMACS | Feature | New                | Normal   | expanded ensemble -- Adaptive Integration Method   | Christopher Mirabzadeh | 07/11/2016 08:01 PM |                |
| 1864 | GROMACS | Feature | New                | Normal   | write tng files with energies  | Magnus Lundborg        | 07/11/2016 08:00 PM |                |
| 2001 | GROMACS | Feature | New                | Normal   | add MPI info to the mdrun log header   |                        | 07/06/2016 05:21 PM |                |
| 1670 | GROMACS | Feature | New                | Normal   | create mdrun option checking mini-tool   |                        | 06/23/2016 04:06 PM |                |
| 1377 | GROMACS | Feature | Feedback wanted    | Low      | Replica exchange if replicas not in ascendent T  | David van der Spoel    | 06/23/2016 03:48 PM |                |

| #    | Project | Tracker | Status      | Priority | Subject  | Assignee            | Updated             | Target version |
|------|---------|---------|-------------|----------|--|---------------------|---------------------|----------------|
| 1900 | GROMACS | Feature | New         | Normal   | Implement some new errors in grompp  |                     | 06/22/2016 05:20 PM |                |
| 1974 | GROMACS | Feature | New         | Normal   | Report atom numbers and types in the error message about missed parameters   |                     | 05/30/2016 09:24 AM |                |
| 1966 | GROMACS | Feature | New         | Low      | Hydrogen mass repartiniog  |                     | 05/25/2016 06:04 PM | future         |
| 1964 | GROMACS | Feature | Accepted    | Normal   | "pull=no" should not produce warnings about "unknown" pull keywords  |                     | 05/20/2016 02:37 PM |                |
| 1953 | GROMACS | Feature | New         | Low      | use more regular polymorphism for GPU code   |                     | 05/06/2016 10:06 PM | future         |
| 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 |                |
| 1885 | GROMACS | Feature | New         | Normal   | DPD Thermostat   |                     | 01/26/2016 10:17 AM |                |
| 1867 | GROMACS | Feature | New         | Normal   | make coupling implementations reversible   |                     | 12/02/2015 07:43 AM |                |
| 1464 | GROMACS | Feature | New         | Normal   | implement PP-PME re-balancing  | Szilárd Páll        | 10/16/2015 08:34 AM | future         |
| 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 |                |
| 1437 | GROMACS | Feature | New         | Normal   | Online help formatting improvements  |                     | 06/04/2015 09:20 PM | future         |
| 1688 | GROMACS | Feature | New         | Low      | g_cluster "middle" is not exactly the same as the definition in the cited paper  |                     | 04/01/2015 05:53 AM |                |
| 1634 | GROMACS | Feature | New         | Normal   | Boxed Molecular Dynamics   |                     | 11/04/2014 04:40 PM |                |
| 1602 | GROMACS | Feature | New         | Low      | gmx order S per slice along all 3 axes   |                     | 09/22/2014 07:25 AM |                |
| 1167 | GROMACS | Feature | New         | Low      | trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values | David van der Spoel | 06/23/2014 04:13 AM | future         |
| 731  | GROMACS | Feature | New         | Normal   | pdb2gmx should warn about missing residues when bonds are too long   |                     | 06/22/2014 10:55 AM |                |
| 438  | GROMACS | Feature | In Progress | Low      | New tool: g_correl   | Alexey Shvetsov     | 06/20/2014 10:38 AM | future         |
| 1102 | GROMACS | Feature | New         | Normal   | Detect incompletely written itp files  |                     | 06/19/2014 03:23 PM |                |
| 1397 | GROMACS | Feature | New         | Normal   | gmx eneconv -offset 1.998 -dt 2 is broken for large times  | Mark Abraham        | 06/12/2014 01:31 AM | future         |
| 1247 | GROMACS | Feature | New         | Normal   | fix hardcoded references to atom names in analysis tools   | Mark Abraham        | 06/12/2014 01:20 AM | future         |
| 1422 | GROMACS | Feature | New         | Normal   | CSH angle incorrect with GROMOS force field and virtual sites  | David van der Spoel | 06/12/2014 12:01 AM |                |
| 1221 | GROMACS | Feature | Accepted    | Normal   | More generic position mapping for selections   |                     | 06/10/2014 02:58 PM | future         |
| 1518 | GROMACS | Feature | New         | Low      | Enable automatic build checking for newer versions   | Mark Abraham        | 06/04/2014 04:13 PM | future         |
| 1120 | GROMACS | Feature | New         | Low      | Make build work with multi-cofiguration generators   |                     | 06/03/2014 03:04 PM | future         |
| 843  | GROMACS | Feature | New         | Low      | g_helixorient could benefit from more documentation  | Erik Lindahl        | 05/23/2014 02:02 PM |                |
| 1182 | GROMACS | Feature | New         | Normal   | improve trajectory writing to support parallel I/O   |                     | 05/13/2014 10:42 AM | future         |



| #    | Project                | Tracker | Status          | Priority | Subject  | Assignee         | Updated             | Target version |
|------|------------------------|---------|-----------------|----------|--|------------------|---------------------|----------------|
| 1335 | GROMACS                | Feature | New             | Normal   | Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling | Michael Shirts   | 05/13/2014 10:38 AM | future         |
| 1489 | GROMACS                | Feature | New             | Normal   | Don't solely rely on filename extension  |                  | 04/30/2014 05:23 AM |                |
| 907  | GROMACS                | Feature | Accepted        | Normal   | Add tests for verifying installed headers  |                  | 03/11/2014 09:15 PM | future         |
| 1142 | GROMACS                | Feature | New             | Low      | Synchronizing the differences between point estimation and histogram estimation for free energies                          | Michael Shirts   | 02/20/2014 08:27 PM | future         |
| 895  | GROMACS                | Feature | In Progress     | Normal   | g_rmsf previous frame as reference   |                  | 04/29/2013 07:39 PM | future         |
| 1162 | GROMACS                | Feature | New             | Normal   | Implement gb_saltconc  | Berk Hess        | 02/26/2013 05:33 PM | future         |
| 1104 | GROMACS                | Feature | New             | Low      | Implement dihedral restraints  |                  | 02/06/2013 07:04 PM | future         |
| 1053 | GROMACS                | Feature | In Progress     | Normal   | L-BFGS doesn't use constraints or call do_em_step  | Berk Hess        | 01/18/2013 11:00 AM | future         |
| 760  | GROMACS                | Feature | New             | Low      | Implement rigid body groups  | Berk Hess        | 12/30/2012 06:04 AM | future         |
| 1028 | GROMACS                | Feature | New             | Normal   | Tool to calculate fraction of native contacts during simulation  |                  | 11/01/2012 10:27 PM |                |
| 687  | Support Platforms      | Feature | New             | Normal   | Add content on the front page  |                  | 09/02/2019 01:08 PM |                |
| 2099 | Support Platforms      | Feature | New             | High     | sharing accounts/credentials   |                  | 12/06/2017 08:11 PM |                |
| 694  | Support Platforms      | Feature | Feedback wanted | Normal   | Write instructions/policy for issue handling   | Rossen Apostolov | 05/31/2017 05:41 PM |                |
| 2180 | Support Platforms      | Feature | Fix uploaded    | Low      | releing matrices would work better with a hint for execution   |                  | 05/19/2017 01:02 AM |                |
| 1601 | Support Platforms      | Feature | New             | Normal   | use Git for Jenkins Config   |                  | 05/24/2015 10:59 AM |                |
| 987  | Support Platforms      | Feature | New             | Normal   | Feature wishlist should be moved to Redmine  |                  | 08/03/2012 12:22 PM |                |
| 2188 | TNG trajectory library | Feature | Resolved        | High     | Masses missing from TNG specification  | Magnus Lundborg  | 06/13/2017 05:08 PM |                |
| 1229 | TNG trajectory library | Feature | Resolved        | Normal   | Selection groups   | Magnus Lundborg  | 11/29/2013 04:38 PM | version 1      |
| 1206 | TNG trajectory library | Feature | New             | Low      | XTC Compression  |                  | 10/25/2013 03:43 PM | version 2      |
| 1367 | TNG trajectory library | Feature | In Progress     | Normal   | Break tng_io.c into smaller files  | Magnus Lundborg  | 10/25/2013 10:49 AM | version 1      |
| 1198 | TNG trajectory library | Feature | In Progress     | Normal   | Full documentation for the high-level API  | Magnus Lundborg  | 06/25/2013 10:05 PM | version 2      |
| 1202 | TNG trajectory library | Feature | New             | Normal   | Other hash types   |                  | 06/25/2013 10:02 PM | version 2      |
| 1199 | TNG trajectory library | Feature | New             | Normal   | residue numbering  | Magnus Lundborg  | 04/24/2013 09:33 AM | version 2      |
| 1200 | TNG trajectory library | Feature | New             | Normal   | Field for the PDB format 'segment identifier'  | Magnus Lundborg  | 04/24/2013 09:32 AM | version 2      |
| 1197 | TNG trajectory library | Feature | New             | Normal   | Rework the molecule descriptions   |                  | 03/18/2013 04:16 PM | version 2      |

| #    | Project | Tracker | Status      | Priority | Subject   | Assignee         | Updated             | Target version             |
|------|---------|---------|-------------|----------|---|------------------|---------------------|----------------------------|
| 3317 | GROMACS | Task    | Resolved    | Normal   | Improve testing of the GPU code   | Artem Zhmurov    | 10/06/2020 12:15 PM | 2021-refactoring           |
| 3422 | GROMACS | Task    | Resolved    | Normal   | Implement modular checkpointing for modular simulator                           | Pascal Merz      | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 2859 | GROMACS | Task    | Resolved    | Normal   | Change ArrayRef iterator type from pointer to std::iterator                     |                  | 06/26/2020 06:15 PM |                            |
| 3041 | GROMACS | Task    | Resolved    | Normal   | Remove workaround for gcc bug 58265   |                  | 06/19/2020 04:45 PM |                            |
| 3297 | GROMACS | Task    | Resolved    | Normal   | Require gcc > 5   |                  | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 2998 | GROMACS | Task    | Resolved    | Normal   | Update Python detection   |                  | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 3290 | GROMACS | Task    | Resolved    | Normal   | Require CMake >= 3.12   |                  | 04/14/2020 02:45 PM | 2021-refactoring           |
| 3271 | GROMACS | Task    | Resolved    | Normal   | Adopt PEP-518 for Python package build system configuration.                    |                  | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3154 | GROMACS | Task    | Resolved    | Low      | Update use of Python subprocess for >=3.5                                       |                  | 04/09/2020 10:15 PM |                            |
| 3415 | GROMACS | Task    | New         | Normal   | Port Pre-submit matrix to Gitlab CI   | Szilárd Páll     | 03/23/2020 10:09 AM | 2021-refactoring           |
| 3314 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceStream  | Artem Zhmurov    | 03/20/2020 09:55 AM | 2021-refactoring           |
| 3312 | GROMACS | Task    | In Progress | Normal   | Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers | Artem Zhmurov    | 03/20/2020 09:54 AM | 2021-refactoring           |
| 3446 | GROMACS | Task    | New         | Normal   | apply maintainability updates across all GPU kernels                            | Jonathan Vincent | 03/19/2020 03:31 PM |                            |
| 2792 | GROMACS | Task    | New         | High     | Improvement of PME gather and spread CUDA kernels                               |                  | 03/18/2020 03:57 PM |                            |
| 3445 | GROMACS | Task    | New         | Normal   | create heuristic for c_skipNeutralAtoms   | Jonathan Vincent | 03/17/2020 12:12 PM |                            |
| 3416 | GROMACS | Task    | New         | Normal   | Port post-submit matrix to Gitlab CI  | Joe Jordan       | 03/16/2020 05:50 PM | 2021-refactoring           |
| 3392 | GROMACS | Task    | New         | Low      | Unify box correction for modular simulator                                      | Pascal Merz      | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 2522 | GROMACS | Task    | Resolved    | Normal   | OpenCL context duplication  |                  | 03/11/2020 04:15 PM | future                     |
| 3315 | GROMACS | Task    | Resolved    | Normal   | Platform agnostic DeviceContext   | Artem Zhmurov    | 03/11/2020 04:15 PM | 2021-refactoring           |
| 3421 | GROMACS | Task    | New         | Normal   | Implement client system for global reduction                                    | Pascal Merz      | 03/11/2020 03:31 PM | 2021-infrastructure-stable |
| 3437 | GROMACS | Task    | New         | Normal   | Use builders to prepare modules   | Pascal Merz      | 03/11/2020 07:05 AM | 2021-infrastructure-stable |
| 3419 | GROMACS | Task    | New         | Normal   | Reduce / remove use of legacy t_state objects throughout modular simulator      | Pascal Merz      | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3418 | GROMACS | Task    | New         | Normal   | Infrastructure improvements for modular simulator                               | Pascal Merz      | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3420 | GROMACS | Task    | New         | Normal   | Unify force and shellfc elements for modular simulator                          | Pascal Merz      | 03/10/2020 09:50 PM | 2021-infrastructure-stable |
| 3275 | GROMACS | Task    | New         | Normal   | Document Gitlab CI instead of Jenkins and releng                                | Paul Bauer       | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3370 | GROMACS | Task    | New         | High     | Further improvements to GPU Buffer Ops and Comms                                |                  | 03/04/2020 01:38 PM |                            |
| 3357 | GROMACS | Task    | New         | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs              |                  | 03/04/2020 11:25 AM |                            |
| 1852 | GROMACS | Task    | New         | Normal   | Remove group scheme   |                  | 03/03/2020 09:03 PM | future                     |
| 3279 | GROMACS | Task    | New         | Low      | Provide more advice for building client software                                |                  | 03/02/2020 11:54 AM |                            |
| 3252 | GROMACS | Task    | New         | Normal   | Remove support for 32 bit architectures   |                  | 03/01/2020 02:05 PM |                            |

| #    | Project | Tracker | Status          | Priority | Subject  | Assignee      | Updated             | Target version             |
|------|---------|---------|-----------------|----------|--|---------------|---------------------|----------------------------|
| 3365 | GROMACS | Task    | New             | Low      | consider making GPU bonded work independent from nonbonded                           |               | 03/01/2020 01:11 PM |                            |
| 3366 | GROMACS | Task    | New             | Normal   | Enforce compability of MdModules   |               | 02/28/2020 11:20 AM |                            |
| 3331 | GROMACS | Task    | New             | Low      | Run physical validation tests in Gitlab  | Paul Bauer    | 02/27/2020 11:09 PM | future                     |
| 2723 | GROMACS | Task    | New             | Normal   | Update mdrun-performance.rst to clearly express the nature of task                   | Joe Jordan    | 02/27/2020 11:07 AM | 2020.2                     |
| 3272 | GROMACS | Task    | New             | Normal   | Port complete CI testing to Gitlab   | Paul Bauer    | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 3220 | GROMACS | Task    | New             | Normal   | change rolling pruning scheduling with GPU update                                    |               | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3361 | GROMACS | Task    | New             | Normal   | Gitlab source archive contains files from build directory                            | Paul Bauer    | 02/25/2020 10:13 AM | 2020.2                     |
| 3047 | GROMACS | Task    | Feedback wanted | Normal   | Set required versions for GROMACS 2021   |               | 02/20/2020 11:42 AM |                            |
| 3382 | GROMACS | Task    | Accepted        | Normal   | Split up t_inputrec  |               | 02/17/2020 05:28 PM |                            |
| 3180 | GROMACS | Task    | New             | Normal   | Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.   | Artem Zhmurov | 02/14/2020 12:45 PM | 2021-infrastructure-stable |
| 2965 | GROMACS | Task    | In Progress     | Normal   | Performance of GPU direct communications   |               | 02/14/2020 12:38 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 |
| 2675 | GROMACS | Task    | In Progress     | Normal   | bonded CUDA offload task   |               | 02/12/2020 05:54 PM | 2021                       |
| 2936 | GROMACS | Task    | New             | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types |               | 02/05/2020 03:57 PM | 2021                       |
| 3356 | GROMACS | Task    | New             | Normal   | Expose setting of random seed to API   |               | 01/29/2020 06:16 PM | 2021                       |

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