

## Issues

| #    | Project                | Tracker | Status          | Priority | Subject   | Assignee         | Updated             | Target version             |
|------|------------------------|---------|-----------------|----------|---|------------------|---------------------|----------------------------|
| 2229 | GROMACS                | Feature | New             | High     | Full Object Oriented Modularization of GROMACS MDRUN Codebase   | Mark Abraham     | 08/22/2018 05:03 PM | future                     |
| 2519 | GROMACS                | Task    | New             | High     | Improve/remove PME OpenCL kernel barriers   |                  | 02/15/2019 06:34 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 |                            |
| 2600 | GROMACS                | Bug     | New             | High     | coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype |                  | 08/07/2018 06:50 PM |                            |
| 2637 | GROMACS                | Bug     | New             | High     | gmx solvate tears apart molecules   |                  | 09/11/2018 07:43 PM |                            |
| 2792 | GROMACS                | Task    | New             | High     | Improvement of PME gather and spread CUDA kernels   |                  | 03/18/2020 03:57 PM |                            |
| 3082 | GROMACS                | Task    | New             | High     | move launch/synchronization points to clarify task dependencies   |                  | 12/27/2019 04:21 PM | 2021                       |
| 3210 | GROMACS                | Bug     | New             | High     | rerun does not reproduce dVcoul/dl  |                  | 12/27/2019 10:45 AM |                            |
| 3262 | GROMACS                | Task    | New             | High     | Trjconv - dimer protein-ligand  |                  | 12/20/2019 09:26 PM |                            |
| 3266 | GROMACS                | Bug     | New             | High     | gmx density show wrong symmetrize density profile using -symm?  | Super duper      | 02/28/2020 08:24 AM | 2020.2                     |
| 3370 | GROMACS                | Task    | New             | High     | Further improvements to GPU Buffer Ops and Comms  |                  | 03/04/2020 01:38 PM |                            |
| 2054 | GROMACS                | Feature | Accepted        | High     | PME on GPU  | Aleksei lupinov  | 12/20/2019 12:18 PM | future                     |
| 2071 | GROMACS                | Task    | In Progress     | High     | Low accuracy default settings yield incorrect liquid densities  | Berk Hess        | 01/05/2018 03:32 PM |                            |
| 2915 | GROMACS                | Feature | In Progress     | High     | GPU direct communications   |                  | 02/14/2020 12:48 PM |                            |
| 3093 | GROMACS                | Task    | In Progress     | High     | rework GPU direct halo-exchange related force reduction complexities  |                  | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3189 | GROMACS                | Task    | In Progress     | High     | implement heuristics for switching between different spread/gather kernel layouts                                   | Jonathan Vincent | 01/29/2020 04:18 PM | 2021-infrastructure-stable |
| 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 |
| 2453 | GROMACS                | Task    | Resolved        | High     | PME OpenCL porting effort   | Aleksei lupinov  | 12/20/2019 12:18 PM | 2021                       |
| 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 |                            |
| 2099 | Support Platforms      | Feature | New             | High     | sharing accounts/credentials  |                  | 12/06/2017 08:11 PM |                            |
| 2935 | Support Platforms      | Bug     | New             | High     | redmine issue updates about gerrit uploads stopped working  |                  | 06/11/2019 01:42 PM | current                    |
| 2188 | TNG trajectory library | Feature | Resolved        | High     | Masses missing from TNG specification   | Magnus Lundborg  | 06/13/2017 05:08 PM |                            |
| 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 |                            |
| 665  | GROMACS                | Task    | New             | Normal   | Port existing trajectory analysis tools to use the new framework  |                  | 07/14/2014 11:29 AM | future                     |
| 677  | GROMACS                | Task    | New             | Normal   | Make sure manual uses consistent style throughout   |                  | 06/19/2014 11:49 AM |                            |
| 701  | GROMACS                | Task    | New             | Normal   | Add symbol visibility macros  |                  | 03/02/2019 01:46 AM | future                     |

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|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 731  | GROMACS | Feature | New    | Normal   | pdb2gmx should warn about missing residues when bonds are too long   |                     | 06/22/2014 10:55 AM |                |
| 742  | GROMACS | Feature | New    | Normal   | Enhancing the performance of the free energy code  |                     | 08/26/2019 04:55 PM | future         |
| 765  | GROMACS | Task    | New    | Normal   | Improving serialization of data structures prior to communication  | Mark Abraham        | 05/13/2014 10:04 AM | future         |
| 838  | GROMACS | Task    | New    | Normal   | Improve generic error reporting routines   |                     | 07/11/2016 08:29 PM |                |
| 909  | GROMACS | Task    | New    | Normal   | Reimplement displacement calculation module  |                     | 07/14/2014 11:30 AM | future         |
| 948  | GROMACS | Task    | New    | Normal   | C++ thread synchronization primitives  | Sander Pronk        | 07/11/2016 08:24 PM |                |
| 950  | GROMACS | Feature | New    | Normal   | Path/directory/filename handling in Gromacs  |                     | 07/11/2016 08:24 PM |                |
| 951  | GROMACS | Feature | New    | Normal   | Multiple versions of Gromacs (e.g., single and double) in the same library/binary  |                     | 01/07/2019 02:10 AM | future         |
| 986  | GROMACS | Task    | New    | Normal   | Handling C++ out-of-memory errors  |                     | 12/24/2014 08:42 PM | future         |
| 988  | GROMACS | Task    | New    | Normal   | Definition of "public API"   |                     | 08/28/2019 02:50 PM | future         |
| 996  | GROMACS | Task    | New    | Normal   | C++ MPI Framework  | Roland Schulz       | 07/14/2014 11:53 AM | future         |
| 1017 | GROMACS | Task    | New    | Normal   | C++ Vector/Matrix classes  |                     | 07/11/2016 08:23 PM |                |
| 1028 | GROMACS | Feature | New    | Normal   | Tool to calculate fraction of native contacts during simulation  |                     | 11/01/2012 10:27 PM |                |
| 1102 | GROMACS | Feature | New    | Normal   | Detect incompletely written itp files  |                     | 06/19/2014 03:23 PM |                |
| 1137 | GROMACS | Feature | New    | Normal   | Proposal for integrator framework (do_md) in future GROMACS  | Michael Shirts      | 02/21/2017 12:48 AM | future         |
| 1139 | GROMACS | Feature | New    | Normal   | Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated |                     | 07/11/2016 08:19 PM |                |
| 1140 | GROMACS | Task    | New    | Normal   | Class design for passing options and data  |                     | 07/11/2016 08:19 PM |                |
| 1162 | GROMACS | Feature | New    | Normal   | Implement gb_saltconc  | Berk Hess           | 02/26/2013 05:33 PM | future         |
| 1170 | GROMACS | Task    | New    | Normal   | mdlib reorganization   |                     | 11/17/2016 03:47 PM | future         |
| 1182 | GROMACS | Feature | New    | Normal   | improve trajectory writing to support parallel I/O   |                     | 05/13/2014 10:42 AM | future         |
| 1190 | GROMACS | Bug     | New    | Normal   | Use of FORCE in setting cached variables   | Mark Abraham        | 06/17/2014 06:09 AM |                |
| 1214 | GROMACS | Task    | New    | Normal   | Keep track of important changes for Changelog  | Mark Abraham        | 06/26/2013 11:24 AM |                |
| 1235 | GROMACS | Bug     | New    | Normal   | peptide dihedral angle definitions violate IUPAC   | David van der Spoel | 06/19/2015 12:24 AM | future         |
| 1246 | GROMACS | Task    | New    | Normal   | expanded ensemble .tpr cannot be rerun   | Michael Shirts      | 06/19/2015 01:56 PM |                |
| 1247 | GROMACS | Feature | New    | Normal   | fix hardcoded references to atom names in analysis tools   | Mark Abraham        | 06/12/2014 01:20 AM | future         |
| 1303 | GROMACS | Feature | New    | Normal   | Adding lambda dependent distance for pull code   | Michael Shirts      | 07/11/2016 08:18 PM |                |
| 1323 | GROMACS | Task    | New    | Normal   | determine future of existing tools for   | David van der Spoel | 12/04/2018 11:53 AM |                |
| 1335 | GROMACS | Feature | New    | Normal   | Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling       | Michael Shirts      | 05/13/2014 10:38 AM | future         |
| 1339 | GROMACS | Bug     | New    | Normal   | Center of mass drift with Nose-Hoover, MTK and md-vv   | Michael Shirts      | 06/18/2015 08:53 PM | future         |

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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 1347 | GROMACS | Feature | New    | Normal   | future of tables  | Berk Hess           | 01/09/2020 02:37 PM | future         |
| 1354 | GROMACS | Bug     | New    | Normal   | Constant acceleration NEMD is broken.   | David van der Spoel | 01/09/2019 04:42 PM |                |
| 1397 | GROMACS | Feature | New    | Normal   | gmx eneconv -offset 1.998 -dt 2 is broken for large times   | Mark Abraham        | 06/12/2014 01:31 AM | future         |
| 1411 | GROMACS | Task    | New    | Normal   | Future of thread_mpi  | Mark Abraham        | 02/26/2018 04:56 PM | future         |
| 1422 | GROMACS | Feature | New    | Normal   | CSH angle incorrect with GROMOS force field and virtual sites   | David van der Spoel | 06/12/2014 12:01 AM |                |
| 1437 | GROMACS | Feature | New    | Normal   | Online help formatting improvements   |                     | 06/04/2015 09:20 PM | future         |
| 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 |                |
| 1464 | GROMACS | Feature | New    | Normal   | implement PP-PME re-balancing   | Szilárd Páll        | 10/16/2015 08:34 AM | future         |
| 1489 | GROMACS | Feature | New    | Normal   | Don't solely rely on filename extension   |                     | 04/30/2014 05:23 AM |                |
| 1490 | GROMACS | Task    | New    | Normal   | Usage of forward declarations vs typedef vs #include  | Mark Abraham        | 01/21/2015 10:23 AM |                |
| 1500 | GROMACS | Feature | New    | Normal   | Post-5.0 feature clean-up plan  | Mark Abraham        | 08/26/2019 03:47 PM |                |
| 1505 | GROMACS | Task    | New    | Normal   | improve handling of logging   | Mark Abraham        | 01/02/2019 06:06 PM |                |
| 1515 | GROMACS | Task    | New    | Normal   | improve g_bar output  | Szilárd Páll        | 07/11/2016 08:10 PM |                |
| 1523 | GROMACS | Task    | New    | Normal   | add missing code-paths to CUDA emulation kernel   |                     | 07/11/2016 08:09 PM |                |
| 1562 | GROMACS | Feature | New    | Normal   | introducing a Monte Carlo framework (first application: MC barostat)  | Michael Shirts      | 07/11/2016 08:08 PM |                |
| 1583 | GROMACS | Bug     | New    | Normal   | gmx msd with mol flag requires excessive memory   |                     | 12/18/2017 03:34 PM |                |
| 1587 | GROMACS | Task    | New    | Normal   | improve the configurability of regression tests   |                     | 12/20/2019 12:02 PM | 2021           |
| 1625 | GROMACS | Feature | New    | Normal   | Gromacs Python API  |                     | 03/02/2019 01:44 AM | future         |
| 1634 | GROMACS | Feature | New    | Normal   | Boxed Molecular Dynamics  |                     | 11/04/2014 04:40 PM |                |
| 1635 | GROMACS | Feature | New    | Normal   | Proper Unicode support  |                     | 06/18/2015 08:34 PM |                |
| 1641 | GROMACS | Feature | New    | Normal   | Add toolchain file for Cray systems   |                     | 06/06/2015 11:24 PM |                |
| 1652 | GROMACS | Feature | New    | Normal   | Decide how to represent multiple lambda states internally   | Michael Shirts      | 06/05/2018 03:58 PM |                |
| 1653 | GROMACS | Feature | New    | Normal   | Decide how to represent multiple lambda states in the .top file and how to parse them   | Michael Shirts      | 06/05/2018 03:58 PM |                |
| 1654 | GROMACS | Feature | New    | Normal   | How to carry out movement between chemical end states in a multiple end state framework?  | Michael Shirts      | 07/11/2016 08:05 PM |                |
| 1655 | GROMACS | Bug     | New    | Normal   | g_membed and box type   |                     | 12/09/2014 01:33 PM |                |
| 1658 | GROMACS | Feature | New    | Normal   | Electrostatics treatment for multiple lambda sites  | Berk Hess           | 07/11/2016 08:05 PM |                |
| 1665 | GROMACS | Feature | New    | Normal   | improve free energy non-bonded kernel performance   |                     | 08/26/2019 03:47 PM | future         |
| 1666 | GROMACS | Feature | New    | Normal   | new approach for Verlet-scheme kernel generation  | Erik Lindahl        | 10/08/2018 07:04 PM | future         |

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|------|---------|---------|--------|----------|---|------------------------|---------------------|----------------|
| 1667 | GROMACS | Bug     | New    | Normal   | gmx convert-tpr writes wrong number of mol in output tpr            | David van der Spoel    | 06/27/2016 08:29 PM |                |
| 1670 | GROMACS | Feature | New    | Normal   | create mdrun option checking mini-tool                              |                        | 06/23/2016 04:06 PM |                |
| 1729 | GROMACS | Task    | New    | Normal   | Resolve whether and how to resolve "state" variables stored in .tpr |                        | 05/13/2015 10:48 AM | future         |
| 1730 | GROMACS | Bug     | New    | Normal   | gmx compare does not compare all fields of a .tpr                   |                        | 06/12/2015 09:33 PM | future         |
| 1745 | GROMACS | Task    | New    | Normal   | Moving to C++11 after Gromacs-5.1                                   |                        | 06/01/2016 03:01 PM |                |
| 1758 | GROMACS | Task    | New    | Normal   | Verlet scheme reorganization / modularization                       | Mark Abraham           | 07/20/2015 06:33 PM | future         |
| 1768 | GROMACS | Task    | New    | Normal   | decide future of command-line options vs env vars                   |                        | 11/03/2016 05:51 PM | future         |
| 1770 | GROMACS | Bug     | New    | Normal   | segmentation fault with free energy changes and multiple GPU's      |                        | 07/14/2015 03:24 AM |                |
| 1786 | GROMACS | Task    | New    | Normal   | Python style standards in developer docs                            | Peter Kasson           | 12/26/2019 03:15 PM |                |
| 1793 | GROMACS | Task    | New    | Normal   | cleanup of integration loop   | Mark Abraham           | 10/31/2018 10:49 PM | future         |
| 1811 | GROMACS | Bug     | New    | Normal   | Extrae build issues   |                        | 12/13/2017 03:43 AM |                |
| 1826 | GROMACS | Task    | New    | Normal   | investigate non-optimal results with CPU-GPU balancing on AMD       | Szilárd Páll           | 12/20/2019 12:04 PM | future         |
| 1828 | GROMACS | Task    | New    | Normal   | Exception handling in mdrun   |                        | 10/07/2015 11:36 AM |                |
| 1829 | GROMACS | Task    | New    | Normal   | Future of thread level parallelism                                  |                        | 11/18/2016 05:29 PM |                |
| 1842 | GROMACS | Feature | New    | Normal   | Replace XML with JSON   |                        | 01/18/2018 05:12 PM |                |
| 1849 | GROMACS | Feature | New    | Normal   | expanded ensemble -- Adaptive Integration Method                    | Christopher Mirabzadeh | 07/11/2016 08:01 PM |                |
| 1852 | GROMACS | Task    | New    | Normal   | Remove group scheme   |                        | 03/03/2020 09:03 PM | future         |
| 1854 | GROMACS | Feature | New    | Normal   | Remove all cyclic dependencies                                      |                        | 05/25/2017 08:34 AM |                |
| 1855 | GROMACS | Task    | New    | Normal   | Convert preprocessor use so that symbols are always defined         |                        | 06/28/2016 02:17 PM |                |
| 1862 | GROMACS | Task    | New    | Normal   | Fully replace t_topology by gmx_mtop_t                              |                        | 02/13/2019 04:53 PM |                |
| 1864 | GROMACS | Feature | New    | Normal   | write tng files with energies                                       | Magnus Lundborg        | 07/11/2016 08:00 PM |                |
| 1867 | GROMACS | Feature | New    | Normal   | make coupling implementations reversible                            |                        | 12/02/2015 07:43 AM |                |
| 1876 | GROMACS | Task    | New    | Normal   | Reorganize vector input passed to core MD routines                  |                        | 06/01/2016 01:59 PM | future         |
| 1885 | GROMACS | Feature | New    | Normal   | DPD Thermostat  |                        | 01/26/2016 10:17 AM |                |
| 1900 | GROMACS | Feature | New    | Normal   | Implement some new errors in grompp                                 |                        | 06/22/2016 05:20 PM |                |
| 1934 | GROMACS | Bug     | New    | Normal   | QMMM with ORCA: memory leaks, buffer overflows and much more        |                        | 07/10/2016 09:26 AM |                |
| 1936 | GROMACS | Task    | New    | Normal   | treat default-able mdp fields as strings                            |                        | 04/02/2016 10:32 PM | future         |
| 1947 | GROMACS | Task    | New    | Normal   | Consider fixing corner case in TinyXML2                             | Mark Abraham           | 04/19/2016 01:40 AM |                |
| 1971 | GROMACS | Task    | New    | Normal   | Removing buggy features vs. keeping workflows                       |                        | 01/19/2018 01:36 PM | future         |
| 1972 | GROMACS | Feature | New    | Normal   | external potential modules for refinement against experimental data |                        | 08/22/2018 05:03 PM | future         |

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|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 1973 | GROMACS | Task    | New    | Normal   | OpenCL implementation wish list  |                     | 05/27/2016 03:42 PM |                |
| 1974 | GROMACS | Feature | New    | Normal   | Report atom numbers and types in the error message about missed parameters                               |                     | 05/30/2016 09:24 AM |                |
| 2001 | GROMACS | Feature | New    | Normal   | add MPI info to the mdrun log header   |                     | 07/06/2016 05:21 PM |                |
| 2003 | GROMACS | Task    | New    | Normal   | reconsider various simd flags  |                     | 07/07/2016 11:23 PM |                |
| 2005 | GROMACS | Feature | New    | Normal   | Full Correlation Analysis (FCA) as Trajectory Analysis Module  | Christian Blau      | 02/07/2018 02:19 PM | future         |
| 2009 | GROMACS | Task    | New    | Normal   | improve command-line reporting of useful things  |                     | 07/26/2016 12:54 PM |                |
| 2010 | GROMACS | Task    | New    | Normal   | Use size_t instead of int for indexing   |                     | 07/01/2018 07:57 AM |                |
| 2015 | GROMACS | Feature | New    | Normal   | Auto recovery from dd communication error  |                     | 07/28/2016 03:17 PM |                |
| 2018 | GROMACS | Feature | New    | Normal   | Pulling along a line between given points  |                     | 07/27/2016 09:59 AM |                |
| 2020 | GROMACS | Bug     | New    | Normal   | Possible issue with md-vv integrator   | Mark Abraham        | 03/11/2017 08:30 AM |                |
| 2034 | GROMACS | Feature | New    | Normal   | Unit tests for bonded forces   | David van der Spoel | 06/29/2019 10:22 AM | future         |
| 2035 | GROMACS | Task    | New    | Normal   | A common trajectory analysis data exchange format  |                     | 03/15/2017 05:46 PM | future         |
| 2039 | GROMACS | Bug     | New    | Normal   | mdrun -pinstride defaults are too confusing  |                     | 12/13/2017 04:14 AM |                |
| 2045 | GROMACS | Task    | New    | Normal   | API design and language bindings   | Peter Kasson        | 01/29/2020 03:59 PM |                |
| 2048 | GROMACS | Task    | New    | Normal   | C++11: CUDA dependency on general headers  |                     | 09/07/2016 10:30 PM |                |
| 2053 | GROMACS | Task    | New    | Normal   | refine notation in GPU code  |                     | 12/20/2019 01:04 PM | 2021           |
| 2060 | GROMACS | Feature | New    | Normal   | Convert enum to enum class   |                     | 10/17/2016 05:27 PM |                |
| 2065 | GROMACS | Bug     | New    | Normal   | thread-MPI internal errors   |                     | 11/08/2018 03:43 PM |                |
| 2068 | GROMACS | Feature | New    | Normal   | Access to low level classes  |                     | 03/02/2019 01:37 AM | future         |
| 2080 | GROMACS | Feature | New    | Normal   | add grompp warning for suitability for domain decomposition  |                     | 11/23/2016 03:03 PM |                |
| 2089 | GROMACS | Task    | New    | Normal   | Encourage code review  |                     | 01/10/2017 12:03 AM |                |
| 2090 | GROMACS | Feature | New    | Normal   | redirecting stdout or stderr for testing   | Mark Abraham        | 12/15/2016 03:15 AM |                |
| 2092 | GROMACS | Task    | New    | Normal   | Tests running on GPU, and hardware assignment  |                     | 12/19/2017 05:27 PM | future         |
| 2094 | GROMACS | Bug     | New    | Normal   | Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size |                     | 01/20/2017 04:56 PM |                |
| 2113 | GROMACS | Bug     | New    | Normal   | Google tests and execution order   |                     | 03/05/2018 02:05 PM |                |
| 2115 | GROMACS | Task    | New    | Normal   | trjconv does too many things, and combinations of them work poorly                                       |                     | 10/02/2018 09:04 AM |                |
| 2126 | GROMACS | Feature | New    | Normal   | implement native CUDA support in CMake   |                     | 10/29/2019 09:03 PM |                |
| 2132 | GROMACS | Feature | New    | Normal   | Intermediate code for xvg handling   |                     | 03/08/2017 05:12 PM | future         |
| 2137 | GROMACS | Feature | New    | Normal   | Preliminary refactoring of constraints and update machinery.   | Michael Shirts      | 03/11/2017 08:32 AM | future         |
| 2139 | GROMACS | Feature | New    | Normal   | More precise/explicit documentation conventions  |                     | 01/07/2018 11:54 PM |                |

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| 2158 | GROMACS | Task    | New    | Normal   | consider adding post-submit test that runs PME with 2xNN kernels           |                | 04/19/2017 08:04 PM |                |
| 2169 | GROMACS | Task    | New    | Normal   | remove 'continuation' mdp option   |                | 12/29/2019 10:31 AM | 2021           |
| 2175 | GROMACS | Task    | New    | Normal   | improve clang static analyzer docs further                                 |                | 01/04/2018 04:13 PM | future         |
| 2178 | GROMACS | Task    | New    | Normal   | Move checks for specific warnings to source repo                           |                | 05/12/2017 03:57 PM |                |
| 2185 | GROMACS | Task    | New    | Normal   | add docs on MPI + CUDA w/wo MPS  |                | 05/24/2017 05:17 PM |                |
| 2207 | GROMACS | Feature | New    | Normal   | solvent excluded volume of large molecule with periodic boundary condition |                | 06/16/2017 10:37 AM |                |
| 2208 | GROMACS | Bug     | New    | Normal   | cuFFT linking  |                | 06/30/2017 01:58 PM |                |
| 2216 | GROMACS | Task    | New    | Normal   | GROMACS SIMD acceleration: generation 3                                    | Erik Lindahl   | 07/17/2017 06:57 PM | future         |
| 2220 | GROMACS | Feature | New    | Normal   | report relevant env var behaviour to console                               |                | 07/31/2017 09:40 PM |                |
| 2221 | GROMACS | Task    | New    | Normal   | Avoid preprocessor for SIMD functions                                      |                | 02/21/2018 01:43 PM |                |
| 2224 | GROMACS | Feature | New    | Normal   | Proposed feature: conditional stop   | Vedran Miletic | 12/20/2019 12:11 PM | 2021           |
| 2226 | GROMACS | Feature | New    | Normal   | Harmonise commands for exit in make_ndx and distance                       |                | 08/04/2017 12:24 PM |                |
| 2231 | GROMACS | Bug     | New    | Normal   | convert-tpz aborts when saving subset of the system                        |                | 01/12/2018 03:52 PM |                |
| 2232 | GROMACS | Bug     | New    | Normal   | pdb2gmx can't form special bonds with terminal patched atoms               |                | 12/03/2017 01:35 PM |                |
| 2239 | GROMACS | Feature | New    | Normal   | split libgromacs into base and full  |                | 01/07/2019 01:47 AM |                |
| 2248 | GROMACS | Feature | New    | Normal   | Label all SIMD functions as pure/nodiscard                                 |                | 02/04/2019 04:49 AM |                |
| 2255 | GROMACS | Bug     | New    | Normal   | nstlist override stopped affecting the input parameter listing             |                | 12/17/2017 08:05 AM |                |
| 2282 | GROMACS | Feature | New    | Normal   | Density map toolset  | Christian Blau | 03/21/2019 06:08 PM | future         |
| 2283 | GROMACS | Feature | New    | Normal   | Force distribution analysis  | Bernd Doser    | 10/27/2017 11:44 AM |                |
| 2289 | GROMACS | Feature | New    | Normal   | gmx spatial add ability to perform over multiple reference structures      |                | 11/08/2017 12:31 AM |                |
| 2294 | GROMACS | Task    | New    | Normal   | Require identical hardware on nodes on parallel runs                       |                | 11/19/2017 08:54 PM |                |
| 2304 | GROMACS | Task    | New    | Normal   | Document and propose tracking mdrun heuristics                             |                | 10/03/2018 09:39 PM | future         |
| 2351 | GROMACS | Task    | New    | Normal   | Avoid the SIMD module depending on non-trivial parts of Gromacs            |                | 12/14/2017 02:47 AM | future         |
| 2353 | GROMACS | Task    | New    | Normal   | improve on relative tolerance for constructing tables                      |                | 12/20/2019 12:12 PM | 2021           |
| 2354 | GROMACS | Feature | New    | Normal   | develop configuration file support for control of task layout              |                | 09/19/2018 03:01 PM | future         |
| 2367 | GROMACS | Task    | New    | Normal   | construct pbc_simd less often  |                | 09/24/2018 11:02 PM | future         |
| 2371 | GROMACS | Task    | New    | Normal   | mtop searching needs reconsideration                                       |                | 01/04/2018 11:54 AM | future         |
| 2375 | GROMACS | Task    | New    | Normal   | Clarify execution phases for MD simulation                                 |                | 04/30/2019 12:59 PM |                |
| 2376 | GROMACS | Task    | New    | Normal   | max_mpi_ranks has wrong name   |                | 02/10/2018 11:03 AM |                |
| 2379 | GROMACS | Task    | New    | Normal   | check leftover FIXMEs in r2018   | Szilárd Páll   | 12/31/2018 11:16 AM | future         |
| 2382 | GROMACS | Task    | New    | Normal   | Simplify Doxygen guidelines  |                | 01/13/2018 12:40 AM |                |
| 2383 | GROMACS | Task    | New    | Normal   | Add JSON interface to write and read files                                 | Paul Bauer     | 01/16/2018 02:01 PM | future         |

| #    | Project | Tracker | Status | Priority | Subject   | Assignee     | Updated             | Target version             |
|------|---------|---------|--------|----------|---|--------------|---------------------|----------------------------|
| 2393 | GROMACS | Bug     | New    | Normal   | incorrect error message with omitted command line flag before its argument                    |              | 01/24/2018 11:24 PM |                            |
| 2396 | GROMACS | Task    | New    | Normal   | Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation         | Paul Bauer   | 12/02/2019 01:24 PM | 2021-infrastructure-stable |
| 2402 | GROMACS | Task    | New    | Normal   | PME kernels general performance improvements  |              | 03/26/2018 10:41 AM | future                     |
| 2412 | GROMACS | Task    | New    | Normal   | attempt to do better FFTW planning  |              | 03/15/2018 05:01 PM |                            |
| 2422 | GROMACS | Task    | New    | Normal   | write C kernel for tables in Verlet scheme  |              | 02/26/2018 01:38 PM |                            |
| 2423 | GROMACS | Task    | New    | Normal   | modernize constraints code  | Mark Abraham | 09/19/2018 03:01 PM | future                     |
| 2425 | GROMACS | Task    | New    | Normal   | testing multisim with multiple ranks per simulation   | Mark Abraham | 12/20/2019 12:13 PM | 2021                       |
| 2427 | GROMACS | Bug     | New    | Normal   | gmx select gives syntax error for selection involving evaluating simple arithmetic expression |              | 02/27/2018 05:15 PM |                            |
| 2428 | GROMACS | Feature | New    | Normal   | Add way of selecting interactive arguments of pdb2gmx by string rather than an index          |              | 02/27/2018 06:28 PM |                            |
| 2429 | GROMACS | Feature | New    | Normal   | Add option of periodic chain topology to pdb2gmx  |              | 03/10/2018 01:01 PM |                            |
| 2435 | GROMACS | Task    | New    | Normal   | identify and note about/tune task offload in GPU-bound runs                                   |              | 03/02/2018 04:08 PM |                            |
| 2442 | GROMACS | Task    | New    | Normal   | Port gmx saxs and gmx sans to c++   | Joe Jordan   | 06/28/2018 10:06 PM | future                     |
| 2445 | GROMACS | Task    | New    | Normal   | Decide if/how to check for incompatible user input to mdrun for bonds and vsites              |              | 03/13/2018 02:02 PM |                            |
| 2456 | GROMACS | Task    | New    | Normal   | Add a pull module external potential tests  |              | 03/15/2018 03:02 PM |                            |
| 2460 | GROMACS | Bug     | New    | Normal   | Allow inclusion of user libraries through CMake cache variables                               |              | 03/28/2018 08:47 PM |                            |
| 2462 | GROMACS | Task    | New    | Normal   | consider adding STL misuse tests  |              | 03/23/2018 01:23 AM |                            |
| 2464 | GROMACS | Task    | New    | Normal   | GPU performance goals overview  |              | 03/26/2018 10:42 AM |                            |
| 2469 | GROMACS | Task    | New    | Normal   | implement GPU timer reduction for reporting   |              | 03/27/2018 05:08 PM |                            |
| 2473 | GROMACS | Bug     | New    | Normal   | mdrun sometimes stalls due to large coordinates with no constraints                           |              | 04/04/2018 10:15 PM |                            |
| 2475 | GROMACS | Task    | New    | Normal   | make OpenCL 1st class-citizen in the build system   |              | 12/20/2019 12:14 PM | 2021                       |
| 2480 | GROMACS | Bug     | New    | Normal   | pdb2gmx does not protonate correctly for united-atom Gromos                                   | Mark Abraham | 12/20/2019 12:17 PM | 2021                       |
| 2488 | GROMACS | Task    | New    | Normal   | use MPI non-blocking collectives to overlap pull comm   |              | 04/25/2018 04:19 PM |                            |
| 2490 | GROMACS | Task    | New    | Normal   | evaluate two-step communicators   | Szilárd Páll | 10/03/2018 09:47 PM | future                     |
| 2492 | GROMACS | Task    | New    | Normal   | implement force calculation via ForceProviders containing collections of IForceProvider       | Mark Abraham | 09/19/2018 03:13 PM | future                     |
| 2498 | GROMACS | Task    | New    | Normal   | OpenCL memory pinning/mapping   |              | 12/20/2019 12:18 PM | future                     |
| 2501 | GROMACS | Task    | New    | Normal   | Documentation section on log file contents  | Kevin Boyd   | 10/03/2018 09:48 PM | future                     |
| 2514 | GROMACS | Task    | New    | Normal   | PME OpenCL reductions with intrinsics   |              | 05/31/2018 12:27 AM | future                     |
| 2518 | GROMACS | Task    | New    | Normal   | redesign task-assignment code for OpenCL  |              | 12/20/2019 12:19 PM | future                     |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee            | Updated             | Target version |
|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 2520 | GROMACS | Task    | New    | Normal   | Treat OpenCL kernel width more diligently  |                     | 05/24/2018 06:21 PM |                |
| 2521 | GROMACS | Task    | New    | Normal   | Implement alternating PME/NB wait for OpenCL                                     |                     | 10/15/2018 12:39 PM |                |
| 2524 | GROMACS | Task    | New    | Normal   | struct alignment/packing for OpenCL host & device code                           |                     | 12/20/2019 12:20 PM | future         |
| 2526 | GROMACS | Bug     | New    | Normal   | Bug of gmx hbond   |                     | 05/30/2018 03:12 PM |                |
| 2527 | GROMACS | Task    | New    | Normal   | Rename GpuEventSynchronizer to something more fitting (after mergein PME OpenCL) |                     | 10/30/2018 04:06 AM | future         |
| 2528 | GROMACS | Task    | New    | Normal   | PME GPU tuning   |                     | 12/31/2018 11:18 AM | future         |
| 2530 | GROMACS | Task    | New    | Normal   | consider using CUDA Driver API   |                     | 09/23/2018 11:47 PM | future         |
| 2532 | GROMACS | Task    | New    | Normal   | enable queue priorities in OpenCL  |                     | 05/29/2018 02:29 PM |                |
| 2535 | GROMACS | Task    | New    | Normal   | consider compiling opencl fft kernels once                                       |                     | 05/31/2018 01:33 PM |                |
| 2537 | GROMACS | Task    | New    | Normal   | Simplify PME solve reduction   | Aleksei lupinov     | 12/20/2019 12:21 PM | future         |
| 2538 | GROMACS | Task    | New    | Normal   | organize more of the PME GPU code along task-specific lines                      | Mark Abraham        | 05/31/2018 05:41 PM |                |
| 2544 | GROMACS | Bug     | New    | Normal   | gmx rmsf does not fix periodicity in reference structure                         | David van der Spoel | 08/21/2018 10:36 AM | future         |
| 2545 | GROMACS | Feature | New    | Normal   | Should grompp fix periodicity of input files?                                    | David van der Spoel | 10/03/2018 11:32 PM | future         |
| 2546 | GROMACS | Task    | New    | Normal   | Add more assertions to AWH code  | Viveca Lindahl      | 06/06/2018 11:20 AM | future         |
| 2556 | GROMACS | Feature | New    | Normal   | make default selections suitable for DNA and RNA                                 | Mark Abraham        | 06/20/2018 01:48 PM |                |
| 2563 | GROMACS | Bug     | New    | Normal   | Windows 7 Compilation with GPU support   |                     | 07/02/2018 09:58 AM |                |
| 2564 | GROMACS | Bug     | New    | Normal   | Result Summary Different For Jobs With Different Numbers of Nodes                |                     | 07/05/2018 02:39 PM |                |
| 2567 | GROMACS | Bug     | New    | Normal   | make check fails at test 23 SIMD errors  |                     | 07/10/2018 09:35 AM |                |
| 2570 | GROMACS | Feature | New    | Normal   | Better string formatting and printing  |                     | 05/02/2019 12:20 PM |                |
| 2574 | GROMACS | Feature | New    | Normal   | iForceSchedule Abstraction   | Prashanth Kanduri   | 03/29/2019 05:20 PM | future         |
| 2576 | GROMACS | Bug     | New    | Normal   | gmx potential -correct outputs the wrong potential                               |                     | 07/25/2018 02:58 PM |                |
| 2579 | GROMACS | Feature | New    | Normal   | Add dimensionality option to gmx trjconv -center                                 |                     | 07/19/2018 04:53 PM | future         |
| 2590 | GROMACS | Task    | New    | Normal   | Essential Dynamics as module providing forces                                    | Christian Blau      | 08/22/2018 05:03 PM | future         |
| 2594 | GROMACS | Feature | New    | Normal   | Multi-level GMX API  | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2595 | GROMACS | Task    | New    | Normal   | Reusable Utilities for Schedules   | Prashanth Kanduri   | 02/22/2019 03:48 PM | future         |
| 2596 | GROMACS | Feature | New    | Normal   | Constant potential method  | Benson Muite        | 05/10/2019 09:54 AM |                |
| 2598 | GROMACS | Bug     | New    | Normal   | Tools using read_next_x cannot read TNG files with sanitizers                    |                     | 10/15/2018 01:16 PM | future         |
| 2601 | GROMACS | Feature | New    | Normal   | Free energy calculations, soft-core potential                                    | Vytautas Gapsys     | 02/10/2020 11:29 AM | future         |



| #    | Project | Tracker | Status | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------------------|
| 2603 | GROMACS | Task    | New    | Normal   | Add ability to properly check coordinate files during testing                    | Paul Bauer          | 10/15/2018 01:16 PM | future                     |
| 2606 | GROMACS | Bug     | New    | Normal   | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert |                     | 08/10/2018 01:48 AM |                            |
| 2607 | GROMACS | Bug     | New    | Normal   | Grompp becomes extremely slow when many pull groups are present                  |                     | 08/11/2018 08:54 AM |                            |
| 2608 | GROMACS | Task    | New    | Normal   | Remove code duplication between OpenCL and CUDA                                  |                     | 09/24/2018 12:47 PM |                            |
| 2611 | GROMACS | Bug     | New    | Normal   | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX               |                     | 08/14/2018 07:03 PM |                            |
| 2616 | GROMACS | Task    | New    | Normal   | Model for MD state   |                     | 09/14/2018 05:12 PM |                            |
| 2621 | GROMACS | Task    | New    | Normal   | Fine-Grained API to Describe Force Calculation and Neighbourhood Search          | Prashanth Kanduri   | 08/22/2018 11:36 AM | future                     |
| 2624 | GROMACS | Bug     | New    | Normal   | GPU build system not robust enough   |                     | 09/05/2018 02:00 AM |                            |
| 2644 | GROMACS | Task    | New    | Normal   | Replace compute_globals  | Mark Abraham        | 09/24/2018 05:51 PM | future                     |
| 2645 | GROMACS | Bug     | New    | Normal   | Security   |                     | 09/28/2018 01:16 PM |                            |
| 2649 | GROMACS | Bug     | New    | Normal   | Virial calculation necessary for correct energy calculation on GPU               |                     | 12/17/2018 02:32 PM | future                     |
| 2650 | GROMACS | Task    | New    | Normal   | revise OpenCL stack recommendations  |                     | 12/31/2018 11:19 AM | future                     |
| 2657 | GROMACS | Bug     | New    | Normal   | Biphasic tutorial  |                     | 09/28/2018 10:02 AM |                            |
| 2658 | GROMACS | Task    | New    | Normal   | Secondary structure assignment via DSSP as native gromacs code                   | Christian Blau      | 10/09/2018 04:51 PM | future                     |
| 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                     |
| 2671 | GROMACS | Task    | New    | Normal   | replace constants like M_PI  |                     | 12/20/2019 01:17 PM | future                     |
| 2672 | GROMACS | Task    | New    | Normal   | check & document execution width requirements in OpenCL                          |                     | 12/31/2018 11:20 AM | future                     |
| 2682 | GROMACS | Task    | New    | Normal   | Add MSAN configuration   |                     | 10/09/2018 06:28 PM |                            |
| 2686 | GROMACS | Task    | New    | Normal   | add tests for gpu bonded interactions  |                     | 12/27/2019 04:40 PM | 2021                       |
| 2693 | GROMACS | Bug     | New    | Normal   | Several memory leaks in mdrun  |                     | 12/18/2018 04:22 AM | future                     |
| 2697 | GROMACS | Task    | New    | Normal   | improve FFT library flavor/version reporting                                     |                     | 12/27/2019 04:40 PM | future                     |
| 2699 | GROMACS | Task    | New    | Normal   | Test POWER9  |                     | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 2707 | GROMACS | Bug     | New    | Normal   | Installed OpenCL files include clh file from gpu_utils directory                 |                     | 10/30/2018 04:02 AM |                            |
| 2710 | GROMACS | Feature | New    | Normal   | Separate dwdl for each molecule (of couple-moltype) when running FEP             |                     | 12/27/2019 04:41 PM | 2021                       |
| 2713 | GROMACS | Feature | New    | Normal   | Constant offset for external electric fields                                     |                     | 10/28/2018 12:57 AM |                            |
| 2715 | GROMACS | Feature | New    | Normal   | Avoid requesting the user to recompile gromacs for Intel OpenCL support          |                     | 12/27/2019 04:06 PM | future                     |
| 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                     |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee            | Updated             | Target version             |
|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------------------|
| 2735 | GROMACS | Task    | New    | Normal   | Allow gmx_genrestr to write correct position restraints for molecules after the first molecule | Joe Jordan          | 12/11/2019 09:26 AM | future                     |
| 2739 | GROMACS | Feature | New    | Normal   | Parallel continuous tempering and enhanced sampling feature                                    |                     | 11/13/2018 11:36 PM |                            |
| 2740 | GROMACS | Bug     | New    | Normal   | mdrun reports incorrect error with -bonded gpu without gpu                                     | Mark Abraham        | 11/07/2018 01:59 PM |                            |
| 2754 | GROMACS | Bug     | New    | Normal   | Simulated Tempering seems to be broken   | Michael Shirts      | 02/05/2019 03:58 PM |                            |
| 2763 | GROMACS | Bug     | New    | Normal   | GMXAPI layout / grouping in development docs "modules" page                                    |                     | 12/14/2018 12:49 PM | future                     |
| 2764 | GROMACS | Task    | New    | Normal   | gmxapi version updates for post release-2019   | Eric Irrgang        | 11/21/2018 12:53 PM |                            |
| 2770 | GROMACS | Task    | New    | Normal   | change branch maintenance policy   |                     | 01/16/2020 05:09 PM | 2021                       |
| 2771 | GROMACS | Task    | New    | Normal   | Size independent Hessian for normal mode analysis  |                     | 12/28/2019 10:50 AM | future                     |
| 2773 | GROMACS | Task    | New    | Normal   | improve GPU error handling and make such handling uniform across modules                       |                     | 12/20/2019 01:09 PM | 2021                       |
| 2774 | GROMACS | Feature | New    | Normal   | Refactor shell code into its own integrator  | David van der Spoel | 12/27/2019 04:05 PM | 2021                       |
| 2785 | GROMACS | Bug     | New    | Normal   | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG                     |                     | 11/30/2018 02:36 PM |                            |
| 2787 | GROMACS | Task    | New    | Normal   | allow passing flags to allocateDeviceBuffer  |                     | 12/03/2018 01:54 PM |                            |
| 2788 | GROMACS | Bug     | New    | Normal   | PME will not run on AMD GPU with NVidia GPU present  |                     | 01/03/2019 02:24 PM |                            |
| 2795 | GROMACS | Task    | New    | Normal   | Incorporate regressiontests into core gromacs  |                     | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2806 | GROMACS | Feature | New    | Normal   | SIMD algorithms for ARM SVE // nobonded cluster and others                                     |                     | 12/27/2019 03:59 PM | 2021                       |
| 2833 | GROMACS | Task    | New    | Normal   | Update topology datastructures   | Paul Bauer          | 12/02/2019 01:43 PM | 2021-infrastructure-stable |
| 2835 | GROMACS | Task    | New    | Normal   | Matrix class constraint to upper or lower triangle   |                     | 02/07/2019 02:44 PM |                            |
| 2839 | GROMACS | Task    | New    | Normal   | make module and file naming consistent   |                     | 01/16/2020 05:11 PM | 2021                       |
| 2840 | GROMACS | Feature | New    | Normal   | Test that functionality does not compile that is not supposed to.                              |                     | 01/25/2019 02:35 PM | future                     |
| 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 |                            |
| 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 |                            |
| 2855 | GROMACS | Task    | New    | Normal   | Allow compiling GROMACS without C compiler   |                     | 01/10/2020 12:06 PM |                            |
| 2857 | GROMACS | Task    | New    | Normal   | Clarify recommended function specifies (constexpr, noexcept, pure)                             |                     | 02/04/2019 04:48 AM |                            |
| 2860 | GROMACS | Feature | New    | Normal   | Option for outputting min/max coordinates in gmx traj  |                     | 02/08/2019 12:35 AM |                            |
| 2863 | GROMACS | Task    | New    | Normal   | improve PBC handling   |                     | 03/11/2019 04:28 PM |                            |
| 2864 | GROMACS | Task    | New    | Normal   | Building incompatibilities   | Benson Muite        | 02/19/2019 02:00 PM |                            |
| 2866 | GROMACS | Feature | New    | Normal   | Alternative non-bonded potentials  | David van der Spoel | 03/05/2019 03:50 PM | future                     |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee       | Updated             | Target version             |
|------|---------|---------|--------|----------|--|----------------|---------------------|----------------------------|
| 2869 | GROMACS | Bug     | New    | Normal   | GPU detection error only issued as a note to the log                                       |                | 03/05/2019 04:09 PM |                            |
| 2870 | GROMACS | Bug     | New    | Normal   | GPU detection error message missing from the output  |                | 03/05/2019 03:55 PM |                            |
| 2872 | GROMACS | Bug     | New    | Normal   | gmx solvate and genion topology update   |                | 02/27/2019 10:18 AM |                            |
| 2873 | GROMACS | Bug     | New    | Normal   | Simple way to get last frame from trajectory   |                | 02/28/2019 11:14 PM |                            |
| 2874 | GROMACS | Task    | New    | Normal   | Refactor Gromacs (cluster) neighborlist into separate module                               | Erik Lindahl   | 02/28/2019 11:36 AM |                            |
| 2876 | GROMACS | Bug     | New    | Normal   | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3)                                     | Erik Lindahl   | 03/08/2019 10:32 AM |                            |
| 2877 | GROMACS | Task    | New    | Normal   | use gmx::Options more  | Mark Abraham   | 12/20/2019 01:22 PM | 2021                       |
| 2882 | GROMACS | Task    | New    | Normal   | evaluate different storage layouts for GPU coordinates/changes/forces                      | Szilárd Páll   | 03/07/2019 06:21 PM |                            |
| 2883 | GROMACS | Bug     | New    | Normal   | essentialdynamics fail with Intel MPI  |                | 03/08/2019 03:10 AM |                            |
| 2889 | GROMACS | Task    | New    | Normal   | update grompp warnings for brevity, usefulness and actionability                           | Mark Abraham   | 12/27/2019 04:38 PM | future                     |
| 2897 | GROMACS | Bug     | New    | Normal   | rotation/flex2 can still fail on cpu-only run on OpenCL build                              |                | 04/04/2019 06:24 PM |                            |
| 2902 | GROMACS | Bug     | New    | Normal   | 2019.1 equilibration issue? (Intel 2018u3)   |                | 04/30/2019 08:17 AM |                            |
| 2905 | GROMACS | Task    | New    | Normal   | Add a Jenkins configuration with std library assert  |                | 08/24/2019 05:22 PM |                            |
| 2907 | GROMACS | Bug     | New    | Normal   | Gromacs autocompletion appears to be broken with ZSH                                       |                | 07/16/2019 04:46 AM |                            |
| 2908 | GROMACS | Task    | New    | Normal   | Renaming things in nbxnm   | Berk Hess      | 03/28/2019 10:10 AM |                            |
| 2909 | GROMACS | Task    | New    | Normal   | consider implementing mechanisms to ensure pair lists are not used past their max lifetime |                | 04/03/2019 05:14 PM |                            |
| 2910 | GROMACS | Feature | New    | Normal   | Mixed scaling for 1-4 interactions   |                | 04/10/2019 10:13 PM |                            |
| 2916 | GROMACS | Task    | New    | Normal   | Decide future of symtab  | Paul Bauer     | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 2919 | GROMACS | Task    | New    | Normal   | C++ style guidelines for namespace use   |                | 04/15/2019 01:21 PM |                            |
| 2924 | GROMACS | Bug     | New    | Normal   | Failing version check when reading new tpr file with older gromacs version                 |                | 04/12/2019 10:52 AM |                            |
| 2925 | GROMACS | Task    | New    | Normal   | BasicVector addition operator yields unexpected result when adding scalar                  | Christian Blau | 12/17/2019 10:04 AM | 2021-infrastructure-stable |
| 2928 | GROMACS | Feature | New    | Normal   | Add ability to use expression "count of ATOM_EXPR" in selection statements.                |                | 04/16/2019 04:52 PM |                            |
| 2930 | GROMACS | Feature | New    | Normal   | Limited range for reference group detection in cylinder pulling                            |                | 04/26/2019 05:17 PM |                            |
| 2931 | GROMACS | Feature | New    | Normal   | Tables in Verlet kernels   |                | 04/29/2019 12:01 PM |                            |
| 2933 | GROMACS | Task    | New    | Normal   | Convert walls to a ForceProvider   |                | 04/25/2019 02:43 PM |                            |
| 2936 | GROMACS | Task    | New    | Normal   | introduce check that CPU-GPU transfers/assignments are made between compatible types       |                | 02/05/2020 03:57 PM | 2021                       |
| 2944 | GROMACS | Feature | New    | Normal   | Roadmap for thermostats / barostats in new propagation/integration scheme                  | Michael Shirts | 12/27/2019 04:00 PM | 2021                       |
| 2948 | GROMACS | Bug     | New    | Normal   | SIMD support detected as none on AMD R5 2500U  |                | 05/21/2019 12:58 PM |                            |

| #    | Project | Tracker | Status | Priority | Subject   | Assignee      | Updated             | Target version             |
|------|---------|---------|--------|----------|---|---------------|---------------------|----------------------------|
| 2949 | GROMACS | Bug     | New    | Normal   | cmake fails when building mdrun only  |               | 07/08/2019 10:04 AM |                            |
| 2954 | GROMACS | Bug     | New    | Normal   | genion changes residue numbering  |               | 05/26/2019 12:08 AM |                            |
| 2956 | GROMACS | Feature | New    | Normal   | SAXS resolution   |               | 05/17/2019 09:58 AM |                            |
| 2958 | GROMACS | Bug     | New    | Normal   | Compiling master (to become 2020) using CUDA 9.0                                  |               | 03/02/2020 03:57 PM | 2020.2                     |
| 2961 | GROMACS | Feature | New    | Normal   | How should Python package find GROMACS resources under various circumstances?     |               | 12/09/2019 10:47 AM |                            |
| 2967 | GROMACS | Feature | New    | Normal   | GPU reallocateDeviceBuffer improvements   |               | 01/23/2020 12:15 PM | 2021-refactoring           |
| 2974 | GROMACS | Bug     | New    | Normal   | position-restraints regressiontest fails on intel GPU with OpenCL                 |               | 02/25/2020 03:52 PM | 2020.2                     |
| 2975 | GROMACS | Feature | New    | Normal   | LJ PME calculations on GPUs   |               | 06/12/2019 01:17 PM |                            |
| 2976 | GROMACS | Task    | New    | Normal   | Basic math for Multidimensional arrays  |               | 12/27/2019 04:37 PM | 2021                       |
| 2977 | GROMACS | Feature | New    | Normal   | print DD load balancing improvement   |               | 06/13/2019 10:56 AM |                            |
| 2978 | GROMACS | Bug     | New    | Normal   | Some suggestions about the gmx current tool                                       |               | 06/13/2019 12:41 PM |                            |
| 2980 | GROMACS | Bug     | New    | Normal   | taskassignment fails with unit tests when GPUs and custom number of ranks is used |               | 06/17/2019 05:28 PM |                            |
| 2981 | GROMACS | Bug     | New    | Normal   | segfault in opencl build  |               | 06/18/2019 03:30 AM |                            |
| 2983 | GROMACS | Task    | New    | Normal   | better suited data-types for bonded GPU kernels                                   |               | 07/11/2019 04:32 PM |                            |
| 2984 | GROMACS | Feature | New    | Normal   | More Extensive Selections Examples  | Dallas Warren | 06/18/2019 11:50 PM |                            |
| 2987 | GROMACS | Bug     | New    | Normal   | assess the bonded GPU task assignment default                                     |               | 12/20/2019 01:06 PM | 2021                       |
| 2992 | GROMACS | Task    | New    | Normal   | Split hw_opt in const user options and dynamic settings                           |               | 12/27/2019 04:31 PM | future                     |
| 2993 | GROMACS | Feature | New    | Normal   | Scalar and structured type expression and definitions for API                     | Eric Irrgang  | 10/17/2019 09:55 AM |                            |
| 2994 | GROMACS | Feature | New    | Normal   | Data flow topology in gmxapi 2020   |               | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 2997 | GROMACS | Task    | New    | Normal   | improve performance of alchemical free energy calculations                        |               | 12/27/2019 04:31 PM | 2021                       |
| 2999 | GROMACS | Task    | New    | Normal   | Move all logging in core library and tools to use MDLogger                        |               | 09/06/2019 02:36 PM | 2021-infrastructure-stable |
| 3000 | GROMACS | Bug     | New    | Normal   | CMake "webpage" target does not fail when it should                               |               | 06/25/2019 02:43 PM |                            |
| 3001 | GROMACS | Task    | New    | Normal   | explore simplifying virial and shift force reduction                              |               | 12/27/2019 04:30 PM | 2021                       |
| 3002 | GROMACS | Task    | New    | Normal   | consider splitting bonded work into local/nonlocal                                |               | 06/25/2019 04:06 PM |                            |
| 3003 | GROMACS | Task    | New    | Normal   | implement heuristic fallback to CPU when there is too little work for GPU offload |               | 06/25/2019 04:10 PM |                            |
| 3004 | GROMACS | Task    | New    | Normal   | Move trajectory analysis logging to MDLogger                                      |               | 06/26/2019 09:59 AM |                            |
| 3005 | GROMACS | Task    | New    | Normal   | Move logging in gmx preprocess to MDLogger  |               | 06/26/2019 10:01 AM |                            |
| 3008 | GROMACS | Task    | New    | Normal   | verify block size choice of CUDA bonded kernel                                    |               | 12/27/2019 04:30 PM | 2021                       |
| 3013 | GROMACS | Task    | New    | Normal   | Extend logging levels in MDLogger   |               | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3015 | GROMACS | Task    | New    | Normal   | Create central log handle for calls to gmx_fatal                                  |               | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3016 | GROMACS | Task    | New    | Normal   | intermittent failure of essentialdynamics test                                    |               | 07/18/2019 05:23 PM |                            |

| #    | Project | Tracker | Status | Priority | Subject   | Assignee        | Updated             | Target version             |
|------|---------|---------|--------|----------|---|-----------------|---------------------|----------------------------|
| 3030 | GROMACS | Feature | New    | Normal   | RST style guidelines  |                 | 07/09/2019 03:38 PM |                            |
| 3031 | GROMACS | Task    | New    | Normal   | evaluate the impact of particle order on PME  |                 | 12/27/2019 04:29 PM | 2021                       |
| 3035 | GROMACS | Task    | New    | Normal   | Provide central logger in wrapper binary  | Paul Bauer      | 09/06/2019 02:34 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 |
| 3040 | GROMACS | Task    | New    | Normal   | Refactor Restraint module   |                 | 07/18/2019 03:59 PM |                            |
| 3042 | GROMACS | Bug     | New    | Normal   | core dump error in grompp command   |                 | 10/09/2019 07:30 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 |                            |
| 3054 | GROMACS | Bug     | New    | Normal   | Missing dihedral define   |                 | 08/02/2019 05:47 PM |                            |
| 3057 | GROMACS | Task    | New    | Normal   | re-enable fusion on Power8/9  | Szilárd Páll    | 12/27/2019 04:22 PM | 2021                       |
| 3062 | GROMACS | Task    | New    | Normal   | add twin cut-off mdrun test   |                 | 12/27/2019 04:22 PM | 2021                       |
| 3064 | GROMACS | Task    | New    | Normal   | add test for perturbed bonded forces  |                 | 12/27/2019 04:22 PM | 2021                       |
| 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 |                            |
| 3068 | GROMACS | Bug     | New    | Normal   | Misleading warning on rerun   |                 | 08/26/2019 03:44 PM |                            |
| 3072 | GROMACS | Task    | New    | Normal   | Use gm::index for indexing instead of int   | Christian Blau  | 09/03/2019 04:23 PM | 2021-infrastructure-stable |
| 3073 | GROMACS | Bug     | New    | Normal   | Total potential energy goes crazy, but I don't know why this happens.   |                 | 09/04/2019 07:25 PM |                            |
| 3075 | GROMACS | Bug     | New    | Normal   | Frozen atoms are moving   | Erik Lindahl    | 12/27/2019 10:51 AM |                            |
| 3076 | GROMACS | Task    | New    | Normal   | Selectively activate MdModules during simulation instead of instantiating all of them   | Christian Blau  | 01/17/2020 02:40 PM | 2021-infrastructure-stable |
| 3078 | GROMACS | Task    | New    | Normal   | Allow MD modules to register energy output fields themselves  |                 | 09/06/2019 11:36 AM |                            |
| 3083 | GROMACS | Bug     | New    | Normal   | Listed forces tests failing on ICC19 with AVX2_256 nightly build  |                 | 09/10/2019 11:56 AM |                            |
| 3086 | GROMACS | Bug     | New    | Normal   | gmxapi fails with MPI build of GROMACS 2020   |                 | 09/25/2019 04:18 PM |                            |
| 3088 | GROMACS | Bug     | New    | Normal   | Reference to theory needed for cylindrical pull geometry  |                 | 09/13/2019 11:26 AM |                            |
| 3096 | GROMACS | Task    | New    | Normal   | Multiple time-stepping: correct coupling algorithms, virial calculation and energy output   | Christian Blau  | 09/18/2019 02:18 PM | 2021-infrastructure-stable |
| 3104 | GROMACS | Task    | New    | Normal   | implement GPU DD cycle counting   |                 | 12/27/2019 04:21 PM | 2021                       |
| 3105 | GROMACS | Task    | New    | Normal   | implement GPU PME/PP comm cycle counting  |                 | 12/27/2019 04:20 PM | 2021                       |
| 3114 | GROMACS | Feature | New    | Normal   | Improve GPU update-constraints module   | Artem Zhmurov   | 02/10/2020 04:30 PM | 2021                       |
| 3115 | GROMACS | Feature | New    | Normal   | Device stream manager   |                 | 10/04/2019 09:00 AM |                            |
| 3116 | GROMACS | Bug     | New    | Normal   | regressiontests/freeenergy core dumps on ppc64le  | Paul Bauer      | 10/04/2019 10:52 PM |                            |
| 3117 | GROMACS | Feature | New    | Normal   | Coulomb FEP PME on GPU  | Magnus Lundborg | 02/17/2020 03:58 PM | 2021-infrastructure-stable |

| #    | Project | Tracker | Status | Priority | Subject  | Assignee       | Updated             | Target version             |
|------|---------|---------|--------|----------|--|----------------|---------------------|----------------------------|
| 3119 | GROMACS | Task    | New    | Normal   | clang-tidy coverage of parallelization codepaths                                   |                | 12/27/2019 04:20 PM | 2021                       |
| 3123 | GROMACS | Task    | New    | Normal   | address sanitizer coverage of parallelization code-paths                           |                | 10/05/2019 12:32 AM |                            |
| 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                       |
| 3126 | GROMACS | Feature | New    | Normal   | State propagator GPU data manager  |                | 10/09/2019 02:42 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 |                            |
| 3130 | GROMACS | Task    | New    | Normal   | Interim handling of gmxapi data references.  | Eric Irrgang   | 12/11/2019 11:26 AM | 2021-infrastructure-stable |
| 3131 | GROMACS | Task    | New    | Normal   | support ccache with clang-tidy   | Mark Abraham   | 12/20/2019 08:20 AM | 2021-infrastructure-stable |
| 3132 | GROMACS | Task    | New    | Normal   | gmxapi testing support tools   |                | 10/31/2019 03:35 PM |                            |
| 3135 | GROMACS | Feature | New    | Normal   | Make GPU traits into opaque types  |                | 10/14/2019 10:24 AM |                            |
| 3136 | GROMACS | Bug     | New    | Normal   | gmxapi.operation data flow topology unclear or incomplete                          | Eric Irrgang   | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 3138 | GROMACS | Feature | New    | Normal   | Improve ensemble support in Context specification.                                 |                | 10/15/2019 03:56 PM |                            |
| 3139 | GROMACS | Task    | New    | Normal   | gmxapi Futures should be subscribable  | Eric Irrgang   | 10/15/2019 03:56 PM |                            |
| 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 |
| 3141 | GROMACS | Bug     | New    | Normal   | gmxapi File placeholders missing from beta release                                 | Eric Irrgang   | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3143 | GROMACS | Task    | New    | Normal   | move the non-force accumulation/accounting tasks out of the GPU wait functions     | Szilárd Páll   | 12/27/2019 04:16 PM | 2021                       |
| 3145 | GROMACS | Task    | New    | Normal   | gmxapi.mdrun needs improved (and public) interface for attaching an MD extension.  | Eric Irrgang   | 01/16/2020 04:31 PM | 2021-refactoring           |
| 3147 | GROMACS | Feature | New    | Normal   | gmxapi workflow checkpointing  | Eric Irrgang   | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 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 |                            |
| 3150 | GROMACS | Bug     | New    | Normal   | gmxapi data type annotations are confusing and inadequate                          | Eric Irrgang   | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3152 | GROMACS | Feature | New    | Normal   | Infrastructure and patterns for expressing public interfaces                       |                | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3162 | GROMACS | Task    | New    | Normal   | Add virtual site support to GPU version of update-constraints.                     | Artem Zhmurov  | 01/23/2020 11:52 AM | 2021-infrastructure-stable |
| 3165 | GROMACS | Bug     | New    | Normal   | task assignment silent abort   |                | 10/18/2019 07:46 PM |                            |
| 3166 | GROMACS | Bug     | New    | Normal   | Compilation failing on Ubuntu 19.04 with Cuda 10.1                                 |                | 10/19/2019 09:13 PM |                            |
| 3171 | GROMACS | Task    | New    | Normal   | schedule CPU H2D force contribution in separate stream                             |                | 12/20/2019 08:33 AM | 2021-infrastructure-stable |
| 3172 | GROMACS | Feature | New    | Normal   | QM/MM Interface with CP2K  | Dmitry Morozov | 01/17/2020 12:18 PM | future                     |
| 3177 | GROMACS | Feature | New    | Normal   | Spack package management support   |                | 11/06/2019 06:37 PM |                            |
| 3179 | GROMACS | Feature | New    | Normal   | Clarify access to parallel data outputs  | Eric Irrgang   | 10/26/2019 12:23 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 |

| #    | Project | Tracker | Status | Priority | Subject   | Assignee       | Updated             | Target version             |
|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3181 | GROMACS | Task    | New    | Normal   | consolidate task assignment and workload data initialization  |                | 10/28/2019 02:53 PM |                            |
| 3185 | GROMACS | Task    | New    | Normal   | Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels.                                     |                | 10/30/2019 11:18 AM |                            |
| 3187 | GROMACS | Task    | New    | Normal   | Template updated PME kernels using threads per atom   |                | 10/30/2019 11:33 AM |                            |
| 3194 | GROMACS | Task    | New    | Normal   | consider passing GPU dependency list to both dependency producers and consumers   |                | 11/01/2019 07:10 PM |                            |
| 3196 | GROMACS | Bug     | New    | Normal   | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing  |                | 11/01/2019 11:28 PM |                            |
| 3197 | GROMACS | Bug     | New    | Normal   | Rework usage of gitattributes and filter in source code formatting scripts  |                | 11/04/2019 12:50 PM | 2021-infrastructure-stable |
| 3198 | GROMACS | Bug     | New    | Normal   | Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0 |                | 11/06/2019 12:20 PM |                            |
| 3209 | GROMACS | Bug     | New    | Normal   | Interactive molecular dynamics with VMD becomes stuttering after reconnecting   |                | 11/19/2019 11:36 AM |                            |
| 3212 | GROMACS | Task    | New    | Normal   | Update regression tests for new kernel flavours   |                | 11/21/2019 11:50 AM |                            |
| 3213 | GROMACS | Bug     | New    | Normal   | Having a local residuetypes.dat for custom force field  |                | 11/21/2019 09:18 PM |                            |
| 3214 | GROMACS | Bug     | New    | Normal   | Out-of-bounds, overflow and incorrect outputs in gmx spatial  |                | 11/25/2019 04:11 PM |                            |
| 3216 | GROMACS | Task    | New    | Normal   | improve CPU force reductions  | Szilárd Páll   | 12/04/2019 09:24 PM |                            |
| 3220 | GROMACS | Task    | New    | Normal   | change rolling pruning scheduling with GPU update   |                | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3223 | GROMACS | Bug     | New    | Normal   | unit test failures give verify -1   |                | 12/02/2019 11:58 AM |                            |
| 3224 | GROMACS | Task    | New    | Normal   | add regression test case large enough to miscalculated GPU grid launch cases  |                | 12/20/2019 01:18 PM | 2021                       |
| 3227 | GROMACS | Bug     | New    | Normal   | solvate does not check return status of gmx_file_rename   |                | 12/04/2019 01:43 PM |                            |
| 3228 | GROMACS | Bug     | New    | Normal   | gmxapi.commandline_operation should gracefully handle input/output file arguments   | Eric Irrgang   | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3229 | GROMACS | Task    | New    | Normal   | Move checkpointing to the beginning of the MD step  |                | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3233 | GROMACS | Bug     | New    | Normal   | clang-format incorrectly aligning altered function arguments  |                | 12/13/2019 12:41 PM |                            |
| 3235 | GROMACS | Task    | New    | Normal   | Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation   | Christian Blau | 12/12/2019 03:46 PM | 2021-infrastructure-stable |
| 3236 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Pulling support   | Artem Zhmurov  | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 3239 | GROMACS | Bug     | New    | Normal   | GPU DD direct communication with GPU update error with RF   |                | 12/14/2019 05:15 PM |                            |
| 3240 | GROMACS | Bug     | New    | Normal   | segv with GPU DD direct communication with GPU update and -dlb off  |                | 01/15/2020 06:16 PM |                            |
| 3242 | GROMACS | Feature | New    | Normal   | Please do not remove the -nsteps flag   |                | 03/01/2020 01:59 PM |                            |
| 3252 | GROMACS | Task    | New    | Normal   | Remove support for 32 bit architectures   |                | 03/01/2020 02:05 PM |                            |
| 3254 | GROMACS | Task    | New    | Normal   | Remove support for generation of virtual sites to replace aromatic rings in standard residues   |                | 12/19/2019 12:13 PM |                            |

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|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3255 | GROMACS | Task    | New    | Normal   | Move benchmarking options from mdrun to a dedicated tool  |                | 12/19/2019 01:21 PM |                            |
| 3256 | GROMACS | Task    | New    | Normal   | Remove -nsteps option from mdrun  |                | 12/19/2019 12:12 PM |                            |
| 3258 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Enable free energy perturbation   | Artem Zhmurov  | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3264 | GROMACS | Task    | New    | Normal   | Break up MdrunMpiTests  | Paul Bauer     | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 3267 | GROMACS | Task    | New    | Normal   | Document tools  |                | 12/26/2019 03:20 PM | future                     |
| 3268 | GROMACS | Task    | New    | Normal   | add more Intel driver recommendations   |                | 12/26/2019 04:39 PM |                            |
| 3272 | GROMACS | Task    | New    | Normal   | Port complete CI testing to Gitlab  | Paul Bauer     | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug     | New    | Normal   | gmxapi setup.py complains too much  |                | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3274 | GROMACS | Bug     | New    | Normal   | Remove ARM NEON SIMD  |                | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3275 | GROMACS | Task    | New    | Normal   | Document Gitlab CI instead of Jenkins and releng  | Paul Bauer     | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3277 | GROMACS | Feature | New    | Normal   | Allow testing feature that is partly implemented  |                | 12/31/2019 12:44 PM | 2021                       |
| 3281 | GROMACS | Bug     | New    | Normal   | Test data directory GMX_RELEASE_ASSERT triggers   |                | 01/06/2020 08:07 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 |
| 3287 | GROMACS | Task    | New    | Normal   | Deprecate make_ndx, use select instead  |                | 01/23/2020 01:16 PM |                            |
| 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 |
| 3289 | GROMACS | Task    | New    | Normal   | Distinguish identifying and non-identifying inputs to API operations.                           | Eric Irrgang   | 01/10/2020 11:30 AM |                            |
| 3294 | GROMACS | Bug     | New    | Normal   | multiple tests fail on fedora 31  | Paul Bauer     | 02/28/2020 03:12 PM | 2020.2                     |
| 3295 | GROMACS | Feature | New    | Normal   | Expand gmxapi.modify_input use cases.   | Eric Irrgang   | 01/16/2020 05:13 PM | 2021-refactoring           |
| 3298 | GROMACS | Feature | New    | Normal   | start early PP work for first dimension of halo exchange  |                | 03/01/2020 01:36 PM |                            |
| 3300 | GROMACS | Task    | New    | Normal   | Abandon docs/OpenCLTODOList.txt?  |                | 01/15/2020 02:46 PM |                            |
| 3301 | GROMACS | Bug     | New    | Normal   | pdb2gmx adding hydrogen   |                | 01/15/2020 10:17 PM |                            |
| 3304 | GROMACS | Bug     | New    | Normal   | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5 | Michael Shirts | 03/01/2020 03:23 PM | 2020.2                     |
| 3305 | GROMACS | Bug     | New    | Normal   | Case gives FPE with Debug build when GPU update is enabled                                      |                | 01/21/2020 05:44 PM |                            |
| 3306 | GROMACS | Task    | New    | Normal   | Document gmx dos tool more clearly  | Christian Blau | 01/20/2020 02:31 PM | future                     |
| 3307 | GROMACS | Feature | New    | Normal   | General interface for communication between simulation ranks                                    |                | 01/22/2020 03:22 PM | 2021-refactoring           |
| 3308 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Cycle counting for GPU launches   |                | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3309 | GROMACS | Bug     | New    | Normal   | -reprod: checkpoint reading bug and general considerations                                      |                | 02/27/2020 10:45 PM |                            |
| 3324 | GROMACS | Task    | New    | Normal   | Rework CMake handling of GPU code   |                | 01/22/2020 09:52 AM | 2021-refactoring           |
| 3325 | GROMACS | Task    | New    | Normal   | Allow complete re-initialization of a simulation  |                | 01/29/2020 05:13 PM | 2021-refactoring           |
| 3326 | GROMACS | Task    | New    | Normal   | Allow changing task assignment  |                | 01/22/2020 09:44 AM | 2021-refactoring           |
| 3327 | GROMACS | Task    | New    | Normal   | Refactor workload flags   |                | 01/22/2020 09:45 AM | 2021-refactoring           |



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| 3328 | GROMACS | Feature | New    | Normal   | Testing framework for task assignment  |               | 01/22/2020 09:48 AM | 2021-refactoring           |
| 3329 | GROMACS | Task    | New    | Normal   | Extend energy comparison testing framework   |               | 01/22/2020 09:51 AM | 2021-refactoring           |
| 3330 | GROMACS | Task    | New    | Normal   | Compile list of codepaths for testing task assignment  |               | 01/22/2020 10:03 AM | 2021-refactoring           |
| 3332 | GROMACS | Feature | New    | Normal   | gmx helixorient doesn't have a -tu option to change time unit  |               | 01/22/2020 11:57 AM |                            |
| 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 |
| 3334 | GROMACS | Bug     | New    | Normal   | Check for DD when increasing rlist is broken   | Berk Hess     | 02/25/2020 03:28 PM | 2020.2                     |
| 3337 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Merge Leap-Frog, LINC and SETTLE kernels.                                    | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3338 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Do not save intermediate coordinates if there is no constraints              | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3339 | GROMACS | Task    | New    | Normal   | GPU LINC: Warp-level synchronization for coupled constraints   | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3340 | GROMACS | Task    | New    | Normal   | GPU LINC: Move more data to local/shared memory  | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3341 | GROMACS | Task    | New    | Normal   | GPU LINC: Use analytical solution for the matrix A inversion.  | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3342 | GROMACS | Task    | New    | Normal   | GPU SETTLE: Read only one index per water molecule.  | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3343 | GROMACS | Task    | New    | Normal   | GPU SETTLE: Use different ordering for matrices.   | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3344 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Better virial reduction.   | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3345 | GROMACS | Task    | New    | Normal   | GPU update-constraints: Reconsider the naming of coordinates buffer in constraints.                  | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3346 | GROMACS | Task    | New    | Normal   | GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE. | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3348 | GROMACS | Task    | New    | Normal   | GPU LINC and SETTLE: unify virial reduction  | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3350 | GROMACS | Feature | New    | Normal   | GPU update-constraints performance   | 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                       |
| 3352 | GROMACS | Feature | New    | Normal   | GPU update-constraints feature support   | Artem Zhmurov | 01/23/2020 11:59 AM | 2021                       |
| 3353 | GROMACS | Task    | New    | Normal   | Document gmx densmap output  |               | 01/23/2020 12:52 PM |                            |
| 3356 | GROMACS | Task    | New    | Normal   | Expose setting of random seed to API   |               | 01/29/2020 06:16 PM | 2021                       |
| 3357 | GROMACS | Task    | New    | Normal   | Make sure "colvars" interoperates stably and smoothly with gromacs                                   |               | 03/04/2020 11:25 AM |                            |
| 3360 | GROMACS | Task    | New    | Normal   | investigate the future of DD dynamic load balancing with GPU offload                                 |               | 01/29/2020 11:23 AM |                            |
| 3361 | GROMACS | Task    | New    | Normal   | Gitlab source archive contains files from build directory  | Paul Bauer    | 02/25/2020 10:13 AM | 2020.2                     |
| 3362 | GROMACS | Feature | New    | Normal   | gmx traj: add an option to plot each component in a separate file                                    |               | 01/29/2020 06:18 PM |                            |
| 3363 | GROMACS | Feature | New    | Normal   | Improve FEP testing  | Pascal Merz   | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3366 | GROMACS | Task    | New    | Normal   | Enforce compability of MdModules   |               | 02/28/2020 11:20 AM |                            |

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|------|---------|---------|--------|----------|--|-----------------|---------------------|----------------------------|
| 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                     |
| 3369 | GROMACS | Feature | New    | Normal   | Add quote about "the truth"  |                 | 02/05/2020 05:08 PM |                            |
| 3371 | GROMACS | Feature | New    | Normal   | Control FEP using AWH  | Magnus Lundborg | 02/06/2020 02:20 PM | 2021                       |
| 3374 | GROMACS | Feature | New    | Normal   | SimulationInput abstraction  |                 | 03/03/2020 05:32 PM | 2021-refactoring           |
| 3378 | GROMACS | Feature | New    | Normal   | genion usage without stdin (facilitates use in gmx python api)   |                 | 02/13/2020 12:04 PM |                            |
| 3379 | GROMACS | Feature | New    | Normal   | C++ API for simulation input and output  |                 | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3385 | GROMACS | Bug     | New    | Normal   | FindLibStdCpp.cmake - wrong sanity check for clang   |                 | 03/04/2020 06:59 PM |                            |
| 3387 | GROMACS | Bug     | New    | Normal   | Death test bug   |                 | 02/20/2020 05:39 PM |                            |
| 3394 | GROMACS | Feature | New    | Normal   | improve gmxapi error handling  | Eric Irrgang    | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3398 | GROMACS | Bug     | New    | Normal   | Intermittent failure of non-bonded kernels when run using nvprof   |                 | 02/25/2020 12:14 PM |                            |
| 3401 | GROMACS | Feature | New    | Normal   | Policy and procedure for installed headers (public API)  |                 | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3402 | GROMACS | Feature | New    | Normal   | Clarify distinction between public API documentation and developer docs.   |                 | 02/26/2020 04:16 PM | 2021-infrastructure-stable |

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