

## Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
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	
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
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	

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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, MTTK and md-vv	Michael Shirts	06/18/2015 08:53 PM	future
1347	GROMACS	Feature	New	Normal	future of tables	Berk Hess	01/09/2020 02:37 PM	future
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
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	

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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
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	

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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
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	

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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	
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	

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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
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	

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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
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 mergin PME OpenCL)		10/30/2018 04:06 AM	future
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
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	

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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
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



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
2735	GROMACS	Task	New	Normal	Allow gmx_genrest 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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
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 gmx::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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelizaton codepaths		12/27/2019 04:20 PM	2021
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
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 Irgang	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 ino opaque types		10/14/2019 10:24 AM	
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irgang	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 Irgang	10/15/2019 03:56 PM	
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irgang	12/10/2019 02:00 PM	2021-infrastructure-stable
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irgang	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 Irgang	01/16/2020 04:31 PM	2021-refactoring
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irgang	10/15/2019 06:21 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 PM	2021-infrastructure-stable
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	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
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, LINCS 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 LINCS: Warp-level synchronization for coupled constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3340	GROMACS	Task	New	Normal	GPU LINCS: Move more data to local/shared memory	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3341	GROMACS	Task	New	Normal	GPU LINCS: Use analytical solution for the matrix A inversion.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
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 LINCS 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



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
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	FindLibStdCmake - 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
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 PM	2021
3411	GROMACS	Bug	New	Normal	Nightly master release build failure		03/06/2020 11:44 AM	2021-infrastructure-stable
3412	GROMACS	Bug	New	Normal	Domain decomposition problems with Gromacs >2018		03/06/2020 04:10 PM	
3415	GROMACS	Task	New	Normal	Port Pre-submit matrix to Gitlab CI	Szilárd Páll	03/23/2020 10:09 AM	2021-refactoring
3416	GROMACS	Task	New	Normal	Port post-submit matrix to Gitlab CI	Joe Jordan	03/16/2020 05:50 PM	2021-refactoring
3417	GROMACS	Feature	New	Normal	Make modular simulator feature-complete	Pascal Merz	03/23/2020 03:57 AM	2021-infrastructure-stable
3418	GROMACS	Task	New	Normal	Infrastructure improvements for modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3419	GROMACS	Task	New	Normal	Reduce / remove use of legacy t_state objects throughout modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3420	GROMACS	Task	New	Normal	Unify force and shellfc elements for modular simulator	Pascal Merz	03/10/2020 09:50 PM	2021-infrastructure-stable
3421	GROMACS	Task	New	Normal	Implement client system for global reduction	Pascal Merz	03/11/2020 03:31 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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

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