

## Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2647	GROMACS	Bug	New	Normal	Removing CGLO_TEMPERATURE flag in MD Setup leads to fatal error because of missing bonded interactions		09/21/2018 12:37 AM	2019
2645	GROMACS	Bug	New	Normal	Security		09/21/2018 03:22 PM	
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/17/2018 09:55 AM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2642	GROMACS	Bug	Accepted	Normal	mdrun with SIMD triggers floating point exceptions	Mark Abraham	09/21/2018 05:18 PM	2019
2641	GROMACS	Feature	Feedback wanted	Normal	Possible l-bfgs improvements	David van der Spoel	09/12/2018 10:59 PM	
2640	GROMACS	Bug	Resolved	High	coul-lambda affects the pressure computation of a ligand with zero partial charge	Berk Hess	09/11/2018 03:15 PM	2018.4
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2636	GROMACS	Bug	Resolved	Low	DD code writes to terminals too much	Mark Abraham	09/11/2018 04:45 PM	2019
2635	GROMACS	Bug	Feedback wanted	Normal	Failing to detect GPUs should not write to terminals	Mark Abraham	09/12/2018 11:01 PM	2019
2634	GROMACS	Bug	Accepted	Low	rerun function returns fault error on trajectory which passed gmx check		09/05/2018 01:36 AM	2018.4
2632	GROMACS	Bug	New	Low	cmake can define incorrect hwloc version with cross-compilation enabled		09/01/2018 09:37 PM	2018.4
2630	GROMACS	Task	New	Normal	gmxapi integration testing		09/01/2018 04:33 PM	
2629	GROMACS	Task	New	Normal	stabilise testing matrices for GROMACS 2019		09/04/2018 10:44 PM	2019-beta1
2628	GROMACS	Bug	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 PM	
2626	GROMACS	Feature	Fix uploaded	Normal	Enable outputting average pull forces (and positions)	Magnus Lundborg	08/23/2018 04:10 PM	2019
2625	GROMACS	Bug	Fix uploaded	Normal	Movement of pull group COM atom of a large pull group can cause crashes	Magnus Lundborg	08/23/2018 11:27 AM	2019
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2623	GROMACS	Task	New	Normal	Allow extensible MDModules and forceProviders.		08/22/2018 05:05 PM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	future
2620	GROMACS	Feature	New	Normal	MD signaling API		08/28/2018 07:10 PM	
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2615	GROMACS	Feature	New	Normal	Switch to Python3		09/04/2018 08:02 PM	2019
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
2610	GROMACS	Feature	New	Normal	API status object		09/06/2018 05:35 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2609	GROMACS	Bug	New	Low	Evaluating PMF for angle rotations using gmx WHAM		08/14/2018 03:15 AM	future
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		08/14/2018 09:04 AM	
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2605	GROMACS	Feature	New	Normal	Library access to MD runner		09/14/2018 12:45 PM	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	08/08/2018 05:58 PM	2019
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	08/08/2018 03:32 PM	future
2600	GROMACS	Bug	New	High	coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype		08/07/2018 06:50 PM	
2599	GROMACS	Bug	New	Normal	do_dssp works incorrectly with unknown residues	David van der Spoel	08/27/2018 04:28 PM	2019
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		08/07/2018 05:21 PM	2019
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	08/09/2018 03:50 PM	
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	Prashanth Kanduri	08/03/2018 10:50 AM	future
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	08/02/2018 05:41 PM	future
2590	GROMACS	Task	New	Normal	Essential Dynamics as module providing forces	Christian Blau	08/22/2018 05:03 PM	future
2589	GROMACS	Bug	New	Normal	regressiontests/kernel core dumps on ppc64 (f29)		07/25/2018 05:20 PM	
2587	GROMACS	Feature	New	Normal	Provide Context (e.g. to runner code) to manage client and runtime environment		08/27/2018 02:18 PM	
2586	GROMACS	Feature	New	Normal	Versioned libgmxapi target for build, install, headers, docs		08/09/2018 01:21 PM	
2585	GROMACS	Feature	New	Normal	Infrastructure supporting external API		09/13/2018 04:24 PM	
2584	GROMACS	Bug	Accepted	Normal	regressiontests/complex fails on i686		09/20/2018 09:25 PM	2018.4
2582	GROMACS	Bug	Blocked, need info	Normal	Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6	Szilárd Páll	07/23/2018 07:46 PM	
2581	GROMACS	Feature	New	Normal	User interface for hybrid Monte Carlo		07/20/2018 03:41 PM	2019
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	
2579	GROMACS	Feature	New	Normal	Add dimensionality option to gmx trjconv -center		07/19/2018 04:53 PM	future
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	08/22/2018 05:03 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2573	GROMACS	Bug	New	High	Different mdp files describing the same change yield different free energy on the same trajectory		07/19/2018 06:52 PM	
2572	GROMACS	Bug	New	Normal	1/viscosity output is wrong in gmx-2018.2, but OK in gmx-5.1.5		07/12/2018 11:18 AM	
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		08/06/2018 06:43 AM	
2569	GROMACS	Task	New	Normal	announce deprecations in GROMACS 2019	Mark Abraham	09/11/2018 04:58 PM	2019
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
2566	GROMACS	Task	Feedback wanted	Normal	Refactor pdb2gmx into c++ framework		08/05/2018 08:08 PM	future
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2562	GROMACS	Bug	Resolved	Normal	Clarify how to do float->int rounding		09/10/2018 09:45 AM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	06/12/2018 01:28 PM	2019
2548	GROMACS	Feature	New	Low	Use metal for GPU acceleration in macOS		07/12/2018 03:30 PM	
2547	GROMACS	Feature	New	Low	Add option of averaging and obtaining error bars for AWH PMFs	Viveca Lindahl	06/06/2018 11:31 AM	future
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 AM	future
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	08/13/2018 02:06 PM	2019
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
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	05/31/2018 05:14 PM	2019
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		05/29/2018 09:04 AM	2019
2529	GROMACS	Task	Resolved	Normal	Improve test timeouts handling	Szilárd Páll	09/21/2018 06:30 PM	2019
2528	GROMACS	Task	New	Normal	PME GPU tuning		05/29/2018 03:08 PM	2019
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)		05/28/2018 12:56 PM	2019
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		05/29/2018 06:51 PM	2019
2522	GROMACS	Task	New	Normal	OpenCL context duplication		05/28/2018 03:13 PM	2019

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		05/25/2018 09:22 PM	
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		05/24/2018 06:05 PM	
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		05/23/2018 04:50 PM	2019
2516	GROMACS	Task	New	Normal	Support PME OpenCL execution width < 16	Aleksei lupinov	05/24/2018 06:08 PM	
2515	GROMACS	Task	Resolved	High	clFFT RocM compatibility problem	Szilárd Páll	09/21/2018 03:28 PM	2019
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 PM	
2512	GROMACS	Bug	New	Normal	Job hanging after a few minutes on BlueGene/Q		07/17/2018 09:19 AM	
2510	GROMACS	Feature	In Progress	Normal	Implement update groups	Berk Hess	05/22/2018 01:06 PM	2019
2505	GROMACS	Task	New	Normal	consider bumping cmake requirement for GROMACS 2020	Roland Schulz	09/19/2018 01:52 PM	2020
2503	GROMACS	Bug	Accepted	Normal	post-submit has warnings	Mark Abraham	05/31/2018 10:23 PM	
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	05/09/2018 08:57 PM	2019
2500	GROMACS	Task	Blocked, need info	Normal	detect and allow linking external clFFT		07/30/2018 12:18 PM	2019
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		05/18/2018 06:36 PM	2019
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2495	GROMACS	Task	New	Normal	replace -noconfout with mdp option	Mark Abraham	09/20/2018 09:12 AM	2019
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2490	GROMACS	Task	New	Normal	evaluate two-step communicators	Szilárd Páll	04/25/2018 02:52 PM	2019
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2484	TNG trajectory library	Bug	Resolved	Normal	Push release tags to github	Magnus Lundborg	04/19/2018 02:33 PM	version 1
2483	GROMACS	Bug	New	Low	gmx dump writes mdp files that can not be parsed by grompp	Paul Bauer	05/25/2018 02:43 PM	
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		09/20/2018 07:43 AM	2020
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	08/21/2018 10:38 AM	2019
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		04/10/2018 04:03 PM	2019
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		08/22/2018 11:23 AM	2018.4
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2461	GROMACS	Task	New	Normal	Expose more info from t_atom to trajectory analysis framework	Joe Jordan	03/22/2018 03:07 PM	future
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
2454	GROMACS	Task	New	Normal	OpenCL infrastructure improvements		05/31/2018 05:00 PM	2019
2453	GROMACS	Task	New	High	PME OpenCL porting effort	Aleksei lupinov	09/20/2018 05:53 PM	2019
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2451	GROMACS	Feature	New	Normal	Linear virtual sites with fixed distance	David van der Spoel	03/19/2018 09:16 AM	2019
2450	GROMACS	Bug	New	Normal	OpenCL runtime version check missing	Szilárd Páll	03/14/2018 08:52 PM	2019
2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2445	GROMACS	Task	New	Normal	Decide if/how to check for incompatible user input to mdrun for bonds and vsites		03/13/2018 02:02 PM	
2442	GROMACS	Task	New	Normal	Port gmx saxs and gmx sans to c++	Joe Jordan	06/28/2018 10:06 PM	future
2438	GROMACS	Task	In Progress	Normal	bump OpenCL requirement to 1.2	Szilárd Páll	03/28/2018 05:32 PM	2019
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2428	GROMACS	Feature	New	Normal	Add way of selecting interactive arguments of pdb2gmx by string rather than an index		02/27/2018 06:28 PM	
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
2426	GROMACS	Feature	In Progress	Normal	Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA)		03/21/2018 12:17 PM	2019
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	03/02/2018 12:42 PM	2019
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
2421	GROMACS	Bug	Resolved	Normal	EwaldUnitTests and SimdUnitTests fail on ppc64le with gcc-8.0.1	Mark Abraham	08/15/2018 11:55 AM	future
2420	GROMACS	Bug	New	Normal	OpenCL implementation not doing device sanity checks		07/30/2018 02:40 PM	2019
2417	GROMACS	Bug	Accepted	Low	Physical validation tests fail with default installation		09/19/2018 11:43 PM	2019
2415	GROMACS	Bug	Blocked, need info	Normal	incorrect runtime assertion catches CUDA API errors from GPU sanity checking	Szilárd Páll	08/15/2018 11:59 AM	2018.4
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2408	GROMACS	Task	New	Normal	device busy error with CC 2.0 and 6.1 in the same run		03/20/2018 12:52 PM	
2404	GROMACS	Bug	Accepted	Normal	Enabling floating point exceptions makes some tests fail		09/12/2018 06:03 PM	2019
2402	GROMACS	Task	New	Normal	PME kernels general performance improvements		03/26/2018 10:41 AM	future
2397	GROMACS	Bug	Feedback wanted	Normal	Difference between single rank and multiple rank when pulling using constraints relative to rest of the system	Berk Hess	09/21/2018 09:17 AM	2018.4
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	02/27/2018 03:30 PM	2019
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	09/19/2018 03:13 PM	2020
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
2391	GROMACS	Task	Accepted	Normal	improve TPI testing coverage	Berk Hess	09/19/2018 03:14 PM	2020
2390	GROMACS	Bug	New	Normal	GROMACS build system should check for valid nvcc flags before use		08/22/2018 11:24 AM	2018.4
2389	GROMACS	Bug	New	Normal	Test don't build with external tinyxml2 version 6	Mark Abraham	02/06/2018 04:45 PM	
2383	GROMACS	Task	New	Normal	Add JSON interface to write and read files	Paul Bauer	01/16/2018 02:01 PM	future
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2379	GROMACS	Task	New	Normal	check leftover FIXMEs in r2018		02/10/2018 10:01 AM	
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		08/09/2018 01:15 PM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2368	GROMACS	Task	In Progress	Normal	update implementation of gmx msd	Kevin Boyd	08/06/2018 10:09 PM	2019
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		12/26/2017 01:53 PM	2019
2362	TNG trajectory library	Bug	New	Normal	tng*_of_particle_nr_get() functions return wrong result for structures with multiple molecule types		12/21/2017 11:51 AM	
2360	GROMACS	Bug	New	Low	error at counter reset with PME-only rank		01/05/2018 12:43 PM	future
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		12/19/2017 08:07 AM	2019
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2344	GROMACS	Task	Resolved	Normal	Agree on standards for different types of output and log files		04/06/2018 05:59 PM	2019
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		09/19/2018 03:12 PM	future
2310	GROMACS	Feature	Accepted	Normal	Let mdrun dump coordinates with non-finite energy		12/26/2017 06:12 AM	2019
2309	GROMACS	Feature	New	Normal	Implement MiMiC QM/MM workflow in the GROMACS core	Viacheslav Bolnykh	01/05/2018 07:09 PM	2019

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2308	GROMACS	Feature	New	Normal	Implement QM/MM updates in GROMACS preprocessor	Viacheslav Bolnykh	01/05/2018 06:19 PM	2019
2307	GROMACS	Feature	New	Normal	Implement the QM/MM functionality in GROMACS	Viacheslav Bolnykh	11/28/2017 05:56 PM	2019
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		04/25/2018 02:40 PM	2019
2297	GROMACS	Task	New	Normal	Transfer parallelisation information from old webpage to new one	Paul Bauer	11/16/2017 09:54 AM	
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2293	GROMACS	Bug	New	Low	libraries target naming in cmake		12/12/2017 02:47 PM	2019
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
2284	GROMACS	Task	New	Low	Hwloc test unstable on Jetson TK1		12/11/2017 12:37 PM	
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	11/08/2017 03:47 PM	future
2281	GROMACS	Task	In Progress	Normal	Represent data on regularly spaced N-dimensional grids.	Christian Blau	11/14/2017 03:56 PM	2019
2269	GROMACS	Feature	New	Low	support some latest-1 versions in Jenkins testing		03/06/2018 11:27 PM	
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
2251	TNG trajectory library	Bug	New	Normal	git release tag for 1.8.0 missing on github	Magnus Lundborg	09/15/2017 11:15 PM	
2250	TNG trajectory library	Bug	New	Normal	tng_io-configVersion.cmake: has no version	Magnus Lundborg	10/23/2017 01:22 PM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		11/12/2017 07:31 PM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		03/06/2018 11:41 PM	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
2231	GROMACS	Bug	New	Normal	convert-tpr aborts when saving subset of the system		01/12/2018 03:52 PM	
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2216	GROMACS	Task	New	Normal	GROMACS SIMD acceleration: generation 3	Erik Lindahl	07/17/2017 06:57 PM	future
2211	GROMACS	Bug	New	Low	gmx writes normal output to stderr		03/05/2018 02:00 PM	future
2208	GROMACS	Bug	New	Normal	cuFFT linking		06/30/2017 01:58 PM	
2207	GROMACS	Feature	New	Normal	solvent excluded volume of large molecule with periodic boundary condition		06/16/2017 10:37 AM	
2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	
2193	GROMACS	Task	New	Normal	OpenCL code modernization assuming v1.2 reqd		03/15/2018 03:34 PM	
2192	GROMACS	Bug	Accepted	Low	grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error	Berk Hess	06/27/2017 11:10 PM	2019
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	
2186	GROMACS	Feature	New	Low	Potential change for logical improvements: move control of constraints purely to the .mdp	Michael Shirts	05/27/2017 10:17 PM	future
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 PM	
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
2180	Support Platforms	Feature	Fix uploaded	Low	releng matrices would work better with a hint for execution		05/19/2017 01:02 AM	
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		05/15/2017 10:42 AM	2019
2168	GROMACS	Task	Feedback wanted	Normal	Design for multiple comparisons against same test reference data		05/08/2017 02:45 PM	future
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
2161	GROMACS	Task	New	Normal	update the way testing matrices are specified	Mark Abraham	09/07/2018 06:53 PM	2019
2158	GROMACS	Task	New	Normal	consider adding post-submit test that runs PME with 2xNN kernels		04/19/2017 08:04 PM	
2149	Support Platforms	Bug	New	Normal	gerrit server excessive CPU usage		04/05/2017 07:25 PM	
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
2146	GROMACS	Task	New	Normal	salvage documentation from old webpage		02/16/2018 03:27 PM	2019
2141	GROMACS	Bug	Feedback wanted	Normal	Each new invocation of mdrun needs it's own setting to use MPI on 28 cores		05/06/2017 08:03 AM	
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 PM	future
2128	GROMACS	Feature	New	Normal	add means to verify at build/run-time that source tarball is not tainted		03/06/2018 10:39 PM	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		02/17/2017 03:47 PM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		02/09/2018 04:13 PM	
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2111	GROMACS	Feature	New	Normal	Implement Gaussian screening of electrostatics		08/21/2018 08:46 AM	
2107	GROMACS	Task	New	Low	Change to clang-format		08/18/2018 09:27 PM	
2101	GROMACS	Feature	New	Low	warning could print the offending line, as well as its number		01/20/2017 03:06 PM	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
2097	GROMACS	Feature	New	Low	Move output of dhdl file entirely toedr, rather than having a separate text dhdl file		01/05/2017 05:21 PM	future
2096	Support Platforms	Bug	New	Normal	Redmine internal error with special characters		05/31/2017 08:48 PM	
2094	GROMACS	Bug	New	Normal	Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size		01/20/2017 04:56 PM	
2092	GROMACS	Task	New	Normal	Tests running on GPU, and hardware assignment		12/19/2017 05:27 PM	future
2091	GROMACS	Feature	New	Normal	CMake support for linking against libgromacs		08/09/2018 10:44 AM	
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2072	GROMACS	Feature	New	Low	target hardware description is silent about the result	Mark Abraham	04/23/2017 12:11 PM	2019
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	09/19/2018 11:41 PM	2019
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2068	GROMACS	Feature	New	Normal	Access to low level classes		10/30/2016 03:13 PM	future
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		05/31/2017 05:30 PM	
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		05/10/2017 03:02 PM	2019
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
2055	GROMACS	Task	New	Low	Wiki registration is broken		01/20/2017 11:31 AM	
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	09/20/2018 05:53 PM	2019

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2053	GROMACS	Task	New	Normal	refine notation in GPU code		12/18/2017 11:12 AM	future
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	07/24/2018 03:53 PM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2035	GROMACS	Task	New	Normal	A common trajectory analysis data exchange format		03/15/2017 05:46 PM	future
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/27/2017 11:12 PM	2019
2030	GROMACS	Task	In Progress	Normal	make the OpenCL nobonded kernels work on Intel iGPU	Szilárd Páll	05/27/2018 11:46 AM	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
2017	GROMACS	Task	In Progress	Normal	Modularize simulation option storage and reading from mdp files	Christian Blau	04/06/2018 06:07 PM	future
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2010	GROMACS	Task	New	Normal	Use size_t instead of int for indexing		07/01/2018 07:57 AM	
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
2005	GROMACS	Feature	New	Normal	Full Correlation Analysis (FCA) as Trajectory Analysis Module	Christian Blau	02/07/2018 02:19 PM	future
2003	GROMACS	Task	New	Normal	reconsider various simd flags		07/07/2016 11:23 PM	
2002	GROMACS	Feature	New	Normal	extend cmake/gmxDetectTargetArchitecture.cmake for ARM and POWER		07/07/2016 09:27 PM	
2001	GROMACS	Feature	New	Normal	add MPI info to the mdrun log header		07/06/2016 05:21 PM	
1994	GROMACS	Feature	New	Low	explore using JIT for CUDA		07/11/2016 10:20 PM	future
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		12/20/2017 06:49 PM	2019
1977	GROMACS	Bug	Feedback wanted	Low	warning: __WORDSIZE not defined		09/21/2018 06:19 PM	2020
1975	GROMACS	Feature	New	Normal	grompp should warn if .mdp define does nothing		06/27/2017 11:32 PM	future
1974	GROMACS	Feature	New	Normal	Report atom numbers and types in the error message about missed parameters		05/30/2016 09:24 AM	
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	
1972	GROMACS	Feature	New	Normal	external potential modules for refinement against experimental data		08/22/2018 05:03 PM	future
1971	GROMACS	Task	New	Normal	Removing buggy features vs. keeping workflows		01/19/2018 01:36 PM	future
1967	Support Platforms	Bug	Resolved	Normal	Documentation pages generated by Jenkins do not render properly		08/27/2016 02:04 AM	
1966	GROMACS	Feature	New	Low	Hydrogen mass repartiniog		05/25/2016 06:04 PM	future
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
1963	GROMACS	Task	New	Low	collect examples of systems where users tried to do something that performed badly	Mark Abraham	08/09/2016 07:30 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1953	GROMACS	Feature	New	Low	use more regular polymorphism for GPU code		05/06/2016 10:06 PM	future
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 PM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	03/17/2018 12:31 AM	2019
1937	GROMACS	Task	New	Low	stop supporting changing CUDA host compiler	Mark Abraham	03/19/2018 11:24 AM	2019
1936	GROMACS	Task	New	Normal	treat default-able mdp fields as strings		04/02/2016 10:32 PM	future
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1925	GROMACS	Task	New	Normal	remove concept of unilateral global communication		05/27/2016 12:04 AM	future
1919	GROMACS	Bug	Accepted	Normal	static linking issues cause by hwloc support		06/27/2017 11:30 PM	2019
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
1902	GROMACS	Feature	Accepted	Low	Add grompp check that non-excluded atoms are not too close to each other in the starting structure		02/15/2016 01:34 PM	
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	12/21/2017 03:20 PM	2019
1879	GROMACS	Task	In Progress	Low	make the GROMACS OpenCL kernel work on Gallium		05/02/2016 12:55 AM	future
1877	GROMACS	Feature	New	Normal	Support reading 3d-grid data from cryo-electron microscopy tomography and X-ray crystallography	Christian Blau	12/11/2015 05:36 PM	future
1876	GROMACS	Task	New	Normal	Reorganize vector input passed to core MD routines		06/01/2016 01:59 PM	future
1868	GROMACS	Task	In Progress	Normal	implement mdrun -rerun better, simplifying do_md	Mark Abraham	09/21/2018 02:04 PM	2019
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1862	GROMACS	Task	New	Normal	Fully replace t_topology by gmx_mtop_t		07/11/2018 11:58 PM	
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
1852	GROMACS	Task	New	Normal	Remove group scheme		05/20/2018 07:28 PM	future
1850	GROMACS	Bug	Accepted	Normal	data race in gmx_parallel_3dfft_init	Berk Hess	07/13/2017 08:53 PM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 PM	
1843	GROMACS	Bug	In Progress	Normal	pbx=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 PM	
1839	GROMACS	Bug	Accepted	Low	pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx		07/09/2016 07:27 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1836	Support Platforms	Bug	New	Normal	Support a way to retrigger part of matrix job		07/22/2017 12:30 AM	
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1828	GROMACS	Task	New	Normal	Exception handling in mdrun		10/07/2015 11:36 AM	
1827	GROMACS	Bug	New	Low	cmake multi-configuration generator support partly broken		12/11/2017 05:20 PM	future
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD		09/16/2015 06:32 PM	
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
1811	GROMACS	Bug	New	Normal	Extrae build issues		12/13/2017 03:43 AM	
1793	GROMACS	Task	New	Normal	cleanup of integration loop	Mark Abraham	09/17/2018 07:21 PM	future
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	07/30/2015 05:45 PM	
1785	GROMACS	Task	New	Low	no pV term written to energy file when pressure coupling is anisotropic		07/26/2015 01:47 PM	future
1782	GROMACS	Feature	New	High	OpenCL runtime/compiler version should be reported in the log...		04/04/2016 07:41 PM	future
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	04/27/2018 06:39 PM	2019
1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 AM	
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future
1758	GROMACS	Task	New	Normal	Verlet scheme reorganization / modularization	Mark Abraham	07/20/2015 06:33 PM	future
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
1744	GROMACS	Feature	New	Low	Add C preprocessor like functionality to mdp files		06/30/2015 09:52 AM	
1732	Support Platforms	Bug	New	Normal	review and extend jenkins tests setups, coverage		05/03/2016 05:30 AM	
1731	Support Platforms	Bug	In Progress	Normal	document jenkins configuration and set up means to track changes		05/31/2017 06:13 PM	
1730	GROMACS	Bug	New	Normal	gmx compare does not compare all fields of a .tpr		06/12/2015 09:33 PM	future
1729	GROMACS	Task	New	Normal	Resolve whether and how to resolve "state" variables stored in .tpr		05/13/2015 10:48 AM	future
1715	GROMACS	Feature	New	Low	improve cycle counting GPU sharing and multi-sim		08/03/2016 12:32 PM	future
1714	GROMACS	Bug	Accepted	Normal	Website: Links to the online manual are broken	Mark Abraham	06/18/2015 04:45 PM	future
1693	GROMACS	Bug	Blocked, need info	Normal	Jenkins Tests seldomly failing		10/17/2017 01:22 PM	
1689	GROMACS	Feature	New	Normal	Add support for [ constraints ] in pdb2gmx		06/16/2015 10:34 PM	
1688	GROMACS	Feature	New	Low	g_cluster "middle" is not exactly the same as the definition in the cited paper		04/01/2015 05:53 AM	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
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	
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	06/27/2017 11:12 PM	2019
1665	GROMACS	Feature	New	Normal	improve free energy non-bonded kernel performance		09/19/2018 03:07 PM	future
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 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	
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	
1652	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states internally	Michael Shirts	06/05/2018 03:58 PM	
1648	GROMACS	Bug	Feedback wanted	Normal	Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges	Michael Shirts	06/25/2015 06:07 AM	
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
1625	GROMACS	Feature	New	Normal	Gromacs Python API		03/08/2017 05:49 PM	future
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 PM	
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	
1601	Support Platforms	Feature	New	Normal	use Git for Jenkins Config		05/24/2015 10:59 AM	
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		07/19/2018 12:53 AM	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 PM	
1551	Support Platforms	Bug	Feedback wanted	Normal	git index.lock issue		05/31/2017 05:37 PM	
1536	TNG trajectory library	Bug	New	Normal	TNG uses incorrect format for size_t on 32bit		06/28/2014 03:56 AM	
1530	GROMACS	Task	New	Low	Offer binary downloads		06/29/2014 02:58 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
1518	GROMACS	Feature	New	Low	Enable automatic build checking for newer versions	Mark Abraham	06/04/2014 04:13 PM	future
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmCIF) support		07/11/2016 08:51 PM	
1509	GROMACS	Task	New	Low	Reduce the distance dependence of shifted potentials for free energies if possible	Michael Shirts	07/11/2016 08:10 PM	
1508	Support Platforms	Task	New	Normal	Update master Jenkins build configurations		06/28/2014 03:59 AM	
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	09/04/2018 09:34 PM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	09/19/2018 03:07 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	
1490	GROMACS	Task	New	Normal	Usage of forward declarations vs typedef vs #include	Mark Abraham	01/21/2015 10:23 AM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1481	GROMACS	Bug	New	Low	g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files	David van der Spoel	06/12/2014 01:37 PM	
1476	GROMACS	Bug	New	Low	Odd behavior with verlet-buffer-drift		05/25/2016 01:45 AM	future
1475	GROMACS	Feature	New	Normal	profiling with Extrae	Rossen Apostolov	09/09/2014 07:16 PM	
1464	GROMACS	Feature	New	Normal	implement PP-PME re-balancing	Szilárd Páll	10/16/2015 08:34 AM	future
1456	GROMACS	Task	New	Low	remove the use of nbat->alloc/free pointers	Szilárd Páll	06/20/2015 11:53 PM	
1448	GROMACS	Bug	New	Normal	multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing)	Mark Abraham	06/23/2016 03:15 PM	
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differencies	Michael Shirts	07/11/2016 08:13 PM	
1437	GROMACS	Feature	New	Normal	Online help formatting improvements		06/04/2015 09:20 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	
1411	GROMACS	Task	New	Normal	Future of thread_mpi	Mark Abraham	02/26/2018 04:56 PM	future
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
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
1373	GROMACS	Task	New	Low	Add missing nbxn tests	Mark Abraham	06/09/2014 08:36 PM	
1367	TNG trajectory library	Feature	In Progress	Normal	Break tng_io.c into smaller files	Magnus Lundborg	10/25/2013 10:49 AM	version 1
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	07/11/2016 08:14 PM	
1347	GROMACS	Feature	New	Normal	future of tables	Mark Abraham	11/03/2017 04:03 PM	2019
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
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
1332	GROMACS	Feature	In Progress	Normal	Supporting multiple end states instead of just A and B	Michael Shirts	06/05/2018 03:58 PM	
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	05/22/2018 05:22 PM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 PM	
1252	TNG trajectory library	Bug	Feedback wanted	Normal	residual ids and atomIDs	Magnus Lundborg	06/12/2013 10:35 AM	version 1
1247	GROMACS	Feature	New	Normal	fix hardcoded references to atom names in analysis tools	Mark Abraham	06/12/2014 01:20 AM	future
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
1242	GROMACS	Feature	Accepted	Normal	Documentation reorganization	Mark Abraham	07/11/2016 08:18 PM	
1235	GROMACS	Bug	New	Normal	peptide dihedral angle definitions violate IUPAC	David van der Spoel	06/19/2015 12:24 AM	future
1229	TNG trajectory library	Feature	Resolved	Normal	Selection groups	Magnus Lundborg	11/29/2013 04:38 PM	version 1
1221	GROMACS	Feature	Accepted	Normal	More generic position mapping for selections		06/10/2014 02:58 PM	future
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1211	GROMACS	Task	New	Low	improve use of preprocessor macros in CUDA kernels	Szilárd Páll	01/12/2015 06:42 PM	future
1206	TNG trajectory library	Feature	New	Low	XTC Compression		10/25/2013 03:43 PM	version 2
1202	TNG trajectory library	Feature	New	Normal	Other hash types		06/25/2013 10:02 PM	version 2
1200	TNG trajectory library	Feature	New	Normal	Field for the PDB format 'segment identifier'	Magnus Lundborg	04/24/2013 09:32 AM	version 2
1199	TNG trajectory library	Feature	New	Normal	residue numbering	Magnus Lundborg	04/24/2013 09:33 AM	version 2
1198	TNG trajectory library	Feature	In Progress	Normal	Full documentation for the high-level API	Magnus Lundborg	06/25/2013 10:05 PM	version 2
1197	TNG trajectory library	Feature	New	Normal	Rework the molecule descriptions		03/18/2013 04:16 PM	version 2
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
1182	GROMACS	Feature	New	Normal	improve trajectory writing to support parallel I/O		05/13/2014 10:42 AM	future
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
1167	GROMACS	Feature	New	Low	trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values	David van der Spoel	06/23/2014 04:13 AM	future
1166	GROMACS	Bug	New	Low	g_order is incorrect for unsaturated carbons	David van der Spoel	06/18/2017 04:40 PM	future
1162	GROMACS	Feature	New	Normal	Implement gb_saltconc	Berk Hess	02/26/2013 05:33 PM	future
1142	GROMACS	Feature	New	Low	Synchronizing the differences between point estimation and histogram estimation for free energies	Michael Shirts	02/20/2014 08:27 PM	future
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
1139	GROMACS	Feature	New	Normal	Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated		07/11/2016 08:19 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1137	GROMACS	Feature	New	Normal	Proposal for integrator framework (do_md) in future GROMACS	Michael Shirts	02/21/2017 12:48 AM	future
1123	GROMACS	Feature	New	Normal	binary incompatibility		07/11/2016 08:52 PM	
1122	GROMACS	Feature	Blocked, need info	Normal	Allow to force pinning	Szilárd Páll	12/31/2017 12:22 AM	
1120	GROMACS	Feature	New	Low	Make build work with multi-cogfiguration generators		06/03/2014 03:04 PM	future
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
1104	GROMACS	Feature	New	Low	Implement dihedral restraints		02/06/2013 07:04 PM	future
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1095	GROMACS	Feature	In Progress	Normal	Fix all-vs-all kernels	Erik Lindahl	03/06/2018 11:19 PM	
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	
1053	GROMACS	Feature	In Progress	Normal	L-BFGS doesn't use constraints or call do_em_step	Berk Hess	01/18/2013 11:00 AM	future
1030	GROMACS	Feature	Fix uploaded	Low	adding -tu option to some analysis tools	Rossen Apostolov	07/11/2016 08:22 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
1026	GROMACS	Feature	New	Low	request for gen_vel to work with multiple temperature coupling groups at different temperatures		11/17/2016 04:39 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
996	GROMACS	Task	New	Normal	C++ MPI Framework	Roland Schulz	07/14/2014 11:53 AM	future
988	GROMACS	Task	New	Normal	Definition of "public API"		11/17/2016 03:48 PM	future
987	Support Platforms	Feature	New	Normal	Feature wishlist should be moved to Redmine		08/03/2012 12:22 PM	
986	GROMACS	Task	New	Normal	Handling C++ out-of-memory errors		12/24/2014 08:42 PM	future
951	GROMACS	Feature	New	Normal	Multiple versions of Gromacs (e.g., single and double) in the same library/binary		01/30/2013 08:08 PM	future
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
920	GROMACS	Task	In Progress	Normal	Add test framework for trajectory analysis modules	Teemu Murtola	07/11/2016 08:27 PM	
909	GROMACS	Task	New	Normal	Reimplement displacement calculation module		07/14/2014 11:30 AM	future
907	GROMACS	Feature	Accepted	Normal	Add tests for verifying installed headers		03/11/2014 09:15 PM	future
895	GROMACS	Feature	In Progress	Normal	g_rmsf previous frame as reference		04/29/2013 07:39 PM	future
889	GROMACS	Feature	New	Normal	pressure annealing		12/30/2012 06:44 AM	future



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
869	GROMACS	Task	In Progress	Normal	Make analysis data histogramming and multipoint data easier to use in parallel	Teemu Murtola	07/11/2016 08:28 PM	
868	GROMACS	Feature	Accepted	Normal	Implement parallelization support to analysis framework		07/11/2016 08:28 PM	
867	GROMACS	Task	In Progress	Normal	Update Doxygen documentation for C++ code	Teemu Murtola	07/11/2016 08:28 PM	
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
837	Support Platforms	Task	Resolved	Low	Consider subproject organization of the Gromacs project		07/14/2014 12:07 PM	
765	GROMACS	Task	New	Normal	Improving serialization of data structures prior to communication	Mark Abraham	05/13/2014 10:04 AM	future
760	GROMACS	Feature	New	Low	Implement rigid body groups	Berk Hess	12/30/2012 06:04 AM	future
742	GROMACS	Feature	New	Normal	Enhancing the performance of the free energy code		04/17/2018 06:51 PM	future
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
701	GROMACS	Task	New	Normal	Add symbol visibility macros		02/15/2014 07:12 PM	future
694	Support Platforms	Feature	Feedback wanted	Normal	Write instructions/policy for issue handling	Rossen Apostolov	05/31/2017 05:41 PM	
687	Support Platforms	Feature	New	Normal	Add content on the front page		01/26/2011 07:29 PM	
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
665	GROMACS	Task	New	Normal	Port existing trajectory analysis tools to use the new framework		07/14/2014 11:29 AM	future
652	GROMACS	Task	Blocked, need info	Normal	Change selection method implementation to use C++		04/23/2017 08:05 PM	future
629	Support Platforms	Task	In Progress	Normal	List of users needs cleanup	Rossen Apostolov	02/21/2018 02:07 PM	
438	GROMACS	Feature	In Progress	Low	New tool: g_correl	Alexey Shvetsov	06/20/2014 10:38 AM	future