Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
620	GROMACS	Bug	Closed	Normal	Total dipole in energy files is incorrect		12/28/2012 08:15 PM	4.6
847	GROMACS	Bug	Rejected	Normal	tpbconv with index file can produce incorrect tpr files		12/29/2012 12:18 AM	4.6
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2720	GROMACS	Bug	Closed	Normal	Normal-mode analysis with vsites or shells works for first molecule of each type only		11/28/2018 03:33 PM	
2843	GROMACS	Bug	Closed	Normal	Building with GMX_BUILD_OWN_FFTW		01/28/2019 04:38 PM	2020
2862	GROMACS	Bug	Closed	Normal	Division by zero in restrained dihedrals		02/28/2020 09:13 AM	2020.1
274	GROMACS	Bug	Closed	Normal	Crashes in mdrun with DD code, not sequential	Berk Hess	01/06/2009 03:35 PM	4.0_rc1
741	GROMACS	Bug	Closed	Normal	tpbconv can not read cpt file	Berk Hess	06/29/2011 06:27 AM	
900	GROMACS	Bug	Closed	High	crash in OpenMP code.	Berk Hess	06/23/2012 06:46 PM	4.6
901	GROMACS	Bug	Closed	Normal	Dispersion correction incorrect with energy minimization	Berk Hess	04/26/2012 08:27 PM	4.5.6
1272	GROMACS	Bug	Closed	Normal	Energy minimization with domain decomposition crashes	Berk Hess	06/16/2015 11:50 PM	
1343	GROMACS	Bug	Closed	Normal	vsiten particles are not integrated	Berk Hess	09/29/2013 03:53 PM	5.0
7	GROMACS	Bug	Closed	High	Environment variable IAMCOOL crashes program luck	David van der Spoel	09/05/2005 05:39 PM	3.3_rc1
45	GROMACS	Bug	Closed	High	pdb2gmx crashes when force field files in workdir	David van der Spoel	02/28/2006 01:58 PM	3.3
50	GROMACS	Bug	Closed	High	grompp -check14 SEGVs	David van der Spoel	02/28/2006 09:51 AM	3.3
53	GROMACS	Bug	Closed	High	Angle definitions maybe wrong in g_chi	David van der Spoel	04/02/2006 05:11 PM	3.3
60	GROMACS	Bug	Closed	High	genion mixes up ions	David van der Spoel	03/30/2006 10:28 AM	CVS
63	GROMACS	Bug	Closed	High	eneconv produces NaN	David van der Spoel	08/21/2006 01:09 PM	3.3
66	GROMACS	Bug	Closed	High	graph problem with distance restraints	David van der Spoel	04/14/2007 03:24 PM	3.3.1
67	GROMACS	Bug	Closed	High	g_rdf has GROMOS atom names hardocoded	David van der Spoel	08/21/2006 01:28 PM	3.3.1
69	GROMACS	Bug	Closed	High	x2top improvements	David van der Spoel	08/20/2006 02:43 PM	3.3.1
71	GROMACS	Bug	Closed	High	grompp takes excessive time for large systems	David van der Spoel	07/21/2007 03:11 PM	3.3.1
80	GROMACS	Bug	Closed	High	bug in avcsix calculation for dispersion correction	David van der Spoel	05/11/2006 08:43 AM	3.3.1
85	GROMACS	Bug	Closed	High	mdrun with PME gives different results with MPI	David van der Spoel	09/11/2007 12:07 PM	3.3.1
103	GROMACS	Bug	Closed	High	Possible problems in g_sas	David van der Spoel	09/21/2007 02:02 PM	3.3.1
206	GROMACS	Bug	Closed	Normal	Protein atom naming in pdb files incorrect	David van der Spoel	10/08/2008 02:38 AM	CVS
440	GROMACS	Bug	Closed	Normal	Double precision man pages are installed as program_d.1	David van der Spoel	09/01/2010 10:22 PM	CVS
520	GROMACS	Bug	Closed	Normal	Editconf with index can not do other things	David van der Spoel	08/31/2010 10:42 AM	CVS
523	GROMACS	Bug	Closed	Normal	g_rms gives nonsense values when the number of atoms differs between tpr and xtc	David van der Spoel	08/31/2010 12:06 PM	CVS
564	GROMACS	Bug	Closed	Normal	g_dipoles has a memory hole	David van der Spoel	09/20/2010 01:51 PM	4.5.1

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608	GROMACS	Bug	Closed	Normal	Molecules with large charge groups give wrong neighborlist	David van der Spoel	11/02/2010 06:18 PM	4.0.7
713	GROMACS	Bug	Closed	Normal	MD with polarization does not work in parallel	David van der Spoel	01/04/2012 01:21 PM	
743	GROMACS	Bug	Closed	Normal	Angular momentum removal incorrect	David van der Spoel	03/05/2012 11:27 AM	4.5.6
972	GROMACS	Bug	Closed	Normal	g_hbond crashes with openmp and -ac	David van der Spoel	11/11/2012 02:01 PM	4.5.6
1183	GROMACS	Bug	Closed	Normal	g_mindist -pi bug with triclinic boxes	David van der Spoel	12/16/2013 05:40 PM	4.5.7
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
1395	GROMACS	Bug	Closed	Normal	rtp errors gromos and opls	David van der Spoel	06/24/2014 08:29 PM	4.6.6
1473	GROMACS	Bug	Closed	Normal	gmx energy -driftcorr broken.	David van der Spoel	07/11/2016 07:48 PM	
1592	GROMACS	Bug	Rejected	Low	Manual of trjconv is unclear about precision.	David van der Spoel	06/22/2015 06:13 AM	
1630	GROMACS	Bug	Closed	Normal	grompp allows to specify vdwtype = PME and dispcorr != no	David van der Spoel	10/24/2014 02:32 PM	5.0.3
1645	GROMACS	Bug	Closed	Normal	Difference in energy with Verlet scheme due to PME dipole correction	David van der Spoel	06/22/2015 06:03 PM	4.6.8
1791	GROMACS	Bug	Closed	Normal	Spurious interactions that should not be there / Table routines work with 1/r leading to NaN.	David van der Spoel	07/11/2016 08:34 PM	
1859	GROMACS	Bug	Closed	Normal	make_ndx does not work	David van der Spoel	01/12/2016 04:23 PM	5.1.2
1860	GROMACS	Bug	Closed	Normal	convert-tpr messes up gmx_mtop_t structure	David van der Spoel	11/24/2015 06:22 PM	5.1.2
1884	GROMACS	Bug	Closed	Normal	gmx_output_env_t not visible from trajectoryanalysis modules	David van der Spoel	12/28/2015 06:16 PM	5.1.2
1996	GROMACS	Bug	Closed	Normal	gmx dos does not work at all	David van der Spoel	06/27/2016 07:27 PM	5.1.3
2011	GROMACS	Bug	Closed	Low	gmx clustsize -mol ignores index file	David van der Spoel	12/31/2017 05:00 PM	
2019	GROMACS	Bug	Closed	Low	gmx velacc lacking documentation	David van der Spoel	12/14/2017 10:27 PM	
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2119	GROMACS	Bug	Closed	Normal	gmx solvate -shell does not add anything	David van der Spoel	12/11/2017 12:17 PM	
2444	GROMACS	Bug	Rejected	Normal	Eneergy minimization crashes due to vsites	David van der Spoel	03/13/2018 02:03 PM	2018.1
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
2641	GROMACS	Bug	Closed	Normal	Possible l-bfgs improvements	David van der Spoel	04/05/2019 04:27 PM	2019.2
2815	GROMACS	Bug	Closed	Normal	gmx msd -mol broken	David van der Spoel	12/26/2018 11:39 AM	2020
2844	GROMACS	Bug	Closed	High	Test SEGV with -DGMX_DOUBLE due to LAPACK	David van der Spoel	02/05/2019 07:01 PM	2020
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
3375	GROMACS	Bug	Closed	Normal	Orires consistency check too strict	David van der Spoel	02/21/2020 08:14 AM	2019.6
3384	GROMACS	Bug	Closed	Normal	Inconsisten labels in distance restraints can crash gmx disre	David van der Spoel	02/24/2020 03:36 PM	2019.6
3386	GROMACS	Bug	Closed	Normal	gmx disre crashed when number of pairs larger than number of restraints	David van der Spoel	02/18/2020 10:17 PM	2019.6
181	GROMACS	Bug	Closed	Normal	Pressure scaling distorts dodecahedron boxes	Erik Lindahl	02/18/2016 11:59 PM	3.3.1

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214	GROMACS	Bug	Closed	Normal	Configure fails in 64 bit	Erik Lindahl	10/08/2008 07:11 AM	4.0_rc1
224	GROMACS	Bug	Closed	Normal	grompp does not process encads topologies correctly	Erik Lindahl	10/08/2008 05:40 PM	4.0_rc1
434	GROMACS	Bug	Closed	Normal	pdb2gmx opens all rtp files	Erik Lindahl	06/14/2010 03:42 PM	CVS
579	GROMACS	Bug	Closed	Normal	nstcalcenergy = -1 leads to wrong pressure	Erik Lindahl	10/05/2010 12:43 PM	4.5.1
1249	GROMACS	Bug	Closed	Normal	no-PBC no-cutoff is broken with SIMD group kernels in 4.6.1	Erik Lindahl	03/04/2015 10:47 PM	4.6.x
1469	GROMACS	Bug	Closed	Normal	sizeof call generates compilation error in src/gromacs/simd/impl_x86_sse2/impl_x86_sse2.h	Erik Lindahl	04/03/2014 07:36 PM	5.0
1502	GROMACS	Bug	Closed	Normal	trjconv incorrect tng defaults	Magnus Lundborg	06/05/2014 04:48 PM	5.0
1510	GROMACS	Bug	Closed	Normal	gmx check and gmx dump do not work for tng files	Magnus Lundborg	07/15/2014 06:45 AM	5.0
1156	GROMACS	Bug	Closed	Normal	mdrun -nt > 1 crashes with old tpr	Michael Shirts	12/16/2013 05:39 PM	4.6.1
720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
2036	GROMACS	Feature	Closed	Normal	gmx solvate should work with molecules		08/23/2016 03:25 PM	2018
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2068	GROMACS	Feature	New	Normal	Access to low level classes		03/02/2019 01:37 AM	future
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 PM	future
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
846	GROMACS	Feature	Closed	Low	Warning messages should be added to programs reducing the precision of coordinates/velocities etc.	David van der Spoel	07/11/2016 08:44 PM	
879	GROMACS	Feature	Closed	Low	Normal modes with vsites and/or shells does not work	David van der Spoel	07/11/2016 08:28 PM	2016
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	
1524	GROMACS	Feature	Closed	Low	More uniform options to programs.	David van der Spoel	08/17/2016 02:25 PM	
1564	GROMACS	Feature	Closed	Low	g_gyrate help text and manual is confusing	David van der Spoel	07/11/2016 07:47 PM	5.0.7
1837	GROMACS	Feature	Closed	High	Design of new table classes	David van der Spoel	03/17/2018 12:31 AM	
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/29/2019 10:22 AM	future
2272	GROMACS	Feature	Closed	Low	pdb2gmx does not accept tips3p as a water model	David van der Spoel	11/28/2017 05:59 PM	2018
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future

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1863	GROMACS	Feature	Closed	Normal	write tng files with velocities from mdrun	Magnus Lundborg	07/11/2016 08:01 PM	2016
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/28/2019 10:50 AM	future
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		12/02/2019 01:44 PM	2021-infrastructure-stable
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
1345	GROMACS	Task	Closed	Low	Charmm - CMAP weirdness in grompp	Erik Lindahl	07/15/2014 06:42 AM	5.0