

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 1170 | GROMACS | Task | New | Normal | mdlib reorganization | | 11/17/2016 03:47 PM | future |
| 1854 | GROMACS | Feature | New | Normal | Remove all cyclic dependencies | | 05/25/2017 08:34 AM | |
| 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 |
| 2132 | GROMACS | Feature | New | Normal | Intermediate code for xvg handling | | 03/08/2017 05:12 PM | future |
| 2568 | GROMACS | Bug | New | Low | gmx editconf -rotate does not rotate the box | | 07/10/2018 10:27 AM | 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 |
| 2931 | GROMACS | Feature | New | Normal | Tables in Verlet kernels | | 04/29/2019 12:01 PM | |
| 1354 | GROMACS | Bug | New | Normal | Constant acceleration NEMD is broken. | David van der Spoel | 01/09/2019 04:42 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 | |
| 2034 | GROMACS | Feature | New | Normal | Unit tests for bonded forces | David van der Spoel | 06/29/2019 10:22 AM | future |
| 2052 | GROMACS | Bug | New | Low | trjconv does not recognize periodic molecules | David van der Spoel | 01/12/2018 11:05 AM | |
| 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 |
| 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 |
| 3049 | GROMACS | Bug | New | Low | gmx nmeig should plot a real infrared spectrum | David van der Spoel | 09/24/2019 03:25 PM | future |
| 1864 | GROMACS | Feature | New | Normal | write tng files with energies | Magnus Lundborg | 07/11/2016 08:00 PM | |
| 720 | GROMACS | Feature | Accepted | Low | permit pdb2gmx to choose a kind of HIS based on proton position | | 11/17/2016 03:51 PM | future |
| 2111 | GROMACS | Feature | In Progress | Normal | Implement Gaussian screening of electrostatics | | 02/23/2019 12:33 PM | |
| 2071 | GROMACS | Task | In Progress | High | Low accuracy default settings yield incorrect liquid densities | Berk Hess | 01/05/2018 03:32 PM | |
| 2451 | GROMACS | Feature | Resolved | Normal | Linear virtual sites with fixed distance | David van der Spoel | 09/16/2019 01:15 PM | |
| 847 | GROMACS | Bug | Rejected | Normal | tpbconv with index file can produce incorrect tpr files | | 12/29/2012 12:18 AM | 4.6 |
| 1592 | GROMACS | Bug | Rejected | Low | Manual of trjconv is unclear about precision. | David van der Spoel | 06/22/2015 06:13 AM | |
| 2444 | GROMACS | Bug | Rejected | Normal | Eneergy minimization crashes due to vsites | David van der Spoel | 03/13/2018 02:03 PM | 2018.1 |
| 1377 | GROMACS | Feature | Feedback wanted | Low | Replica exchange if replicas not in ascendent T | David van der Spoel | 06/23/2016 03:48 PM | |
| 620 | GROMACS | Bug | Closed | Normal | Total dipole in energy files is incorrect | | 12/28/2012 08:15 PM | 4.6 |
| 2036 | GROMACS | Feature | Closed | Normal | gmx solvate should work with molecules | | 08/23/2016 03:25 PM | 2018 |
| 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 | |

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|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 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 hardcoded | 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 |
| 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 |
| 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 |
| 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 |

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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 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 |
| 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 | |
| 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 |
| 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 | |
| 1837 | GROMACS | Feature | Closed | High | Design of new table classes | David van der Spoel | 03/17/2018 12:31 AM | |
| 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 | |
| 2119 | GROMACS | Bug | Closed | Normal | gmx solvate -shell does not add anything | David van der Spoel | 12/11/2017 12:17 PM | |
| 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 |
| 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 |
| 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 |
| 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 | nstcalenergy = -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 |
| 1345 | GROMACS | Task | Closed | Low | Charmm - CMAP weirdness in grompp | Erik Lindahl | 07/15/2014 06:42 AM | 5.0 |

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| 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 |
| 1863 | GROMACS | Feature | Closed | Normal | write tng files with velocities from mdrun | Magnus Lundborg | 07/11/2016 08:01 PM | 2016 |
| 1156 | GROMACS | Bug | Closed | Normal | mdrun -nt > 1 crashes with old tpr | Michael Shirts | 12/16/2013 05:39 PM | 4.6.1 |