Simulation parameters

	~sim_gen_def[] parameters
\simulation_typ{ }	Defines the simulation type to be used. PT or PTMC: Parallel Tempering Monte Carlo MIN: energy minimization EEMC: Equi-energy Monte Carlo PTSTG or PTSTGMC: PTMC with staging transformation NM: Normal Modes NMEN: Elastic normal modes
\replica_number{0}	The highest order replica number in PTMC. Must be an integer ≥ 0. Using 0 defines PTMC with a single replica (conventional MC). Using n defines PTMC with $0, \ldots, n$, $n+1$ replicas.
\total_step_mc{10000}	Total number of steps taken in simulation. Must be an integer ≥ 1.
\local_step_md{1}	Number of molecular dynamics steps taken in each hybrid monte carlo step to generate moves. Only used in cartesian sampling. Must be an integer ≥ 1.
\time_step_md{0.4}	Time step for outer (inter-molecular energies) hybrid Monte Carlo local molecular dynamics move in fs, ≥ 0.
\intra_respa_step{1}	Time step for the inner loop of hybrid Monte Carlo is scaled by the inverse of this value. This is for the evaluation of bond, bond angle and torsional (intra-molecular) energies. Only used in cartesian sampling.
\statistics_freq{200}	Frequency of data printout. Must be an integer ≥ 1.
\prob_eemc_jump{0.15}	For PT simulations. The probability of attempting a PT jump, ≥ 0.

\temperature{300}	Temperature of lowest order replica in PTMC simulation in K, ≥ 0.
\eemc_disk_size{10}	The size of partitions used in EEMC runs.
\burn_in_B{10}	Related to the number of steps replicas are equilibrated. Used in conjunction with \burn_in_N{} below.
\burn_in_N{10}	Used in conjunction with \burn_in_B{}. In PTMC, the i^{th} replica (chain) is equilibrated for \burn_in_B{} + \burn_in_N{} extra number of steps before the $(i-1)^{th}$ chain begins propagating or exchanging with the i^{th} chain. In EEMC, the i^{th} replica (chain) is equilibrated for \burn_in_B{} + \burn_in_N{} extra number of steps before the $(i-1)^{th}$ chain begins propagating. If the EEMC mode further relative equilibration time (defined in number of steps) \burn_in_B{} is applied before exchanges are attempted.
\extend_inter{off}	Defines the excluded interactions in a system of connected atoms or particles (coarse graining). 3bond_conn: 1-2 interactions are excluded 4bond_conn: 1-3 interactions are excluded off (default): 1-4 interactions are excluded
\EEMC_Emin{ }	The lower energy bound of any EEMC partition in Ha.
\EEMC_Emax{ }	The upper energy bound of any EEMC partition Ha.
\write_energy_unit{kcal}	Energy units for data output. (kcal or Ha)
\energy_gap{1.1}	For EEMC, energy levels $E_i = (\text{\energy\_gap\{\}})^i$, are linearly mapped to [\EEMC_Emin{ }, \EEMC_Emax{ }] interval leading to energy levels, $H(i)$, $i = 0, \ldots, n+1$. For PTMC, $\textit{\energy\_gap\{\}}$ defines $H'(i)$, $i = 0, \ldots, n+1$ such that $T(j) = (H'(j+1) - H(j)')/c$, $j = 0, \ldots, n$ and c is chosen such that $T(0)$ corresponds to \temperature{}.

\prop_type{tors}	Propagation type. cart: cartesian sampling tors: torsional sampling bend: bend angle sampling
\prop_tors_sig{1.e-5}	In a Monte Carlo step, the new sampled angle of a conformation is chosen from a normal distribution centered around the original angle, and with standard deviation (σ) defined by \prop_tors_sig{}. The larger σ is, the broader the normal distribution, and the higher the probability that a larger torsional step size is taken. Angle in radians, $0 \leq$ angle $< 2\pi$. Used only in torsional sampling.
\cancel_res_inter{off}	Controls the removal of local non-bonded interactions. neighbor: interactions within a residue/base and those between the residue/base and first neighbor residue/base are turned off. local: interactions within a residue/base are turned off. off (default): no interactions are turned off (none beyond those defined in \extend_inter{}.
\inter_list{none}	Determines the list type used for the calculation of non-bonded interactions. neighbor_list: neighbor list is used to in the intermolecular energy evaluation. lnk_list: linked-list based intermolecular energy evaluation is adopted. none: evaluation of non-bonded interaction considers all possible non-bonded interactions at each step.
\num_procs{1}	Number of processors to be used. Must be 1 for serial version and \replica_number{} + 1 if running in parallel.
\rinter_switch_length{1}	The distance (in Å) over which non-bonded interactions decay to zero.
\prop_tors_type{full}	Type of torsional propagation. full (default): all torsion angles are updated. sidechain: only side chain torsional angles are updated.

\minimize_type{cg}	Minimization approach used. cg (default): conjugate gradient bfgs: Broyden-Fletcher-Goldfarb-Shanno method samc: simulated annealing Monte Carlo stsamc: simulated tempering, simulated annealing MC
\minimize_tol{1.e-7}	The tolerance for minimization acceptance (units are kcal/mol/Å in cartesian space and kcal/mol/rad in torsional space). Minimization stops when the energy gradient is less than \minimize_tol{}/2.
\minimize_report{2}	Output report for minimization routine. 0: No output 1: Reports energies on screen 2 : Reports energies on screen. Trajectory saved in .pos file, the last configuration is output into the .pos_out file.
\energy_report{0}	Energy output report in standard output. 0 (default): no output 1: key energies 2: all energies
\prop_rot_sig{1.e-6}	Similar to \prop_tors_sig{}, but for rotation (angle in radians) for fragments if closure relation is implemented and for independent molecules (e.g. water and ions) with no torsional degree of freedom.
\prop_trans_sig{5.e-6}	Analog to \prop_rot_sig{}, but for translation (in Å) applied on independent molecules (e.g. water and ions) with no torsional degree of freedom and on fragments if closure relation is implemented.
\postprop_minimize{off}	Post-propagation minimization type off (default): none cart: cartesian tors: torsional bend: bend angle bend_tors: bend angle followed by torsional tors_bend: torsional followed by bend angle clos: closure algorithm

\postprop_minimize_itmax{}	Number of steps for post-propagation minimization.
\postprop_minimize_energy{}	Energies included for post-propagation minimization. bond: only bonded atom energies bond_bend: only bonded atom and bend angle energies bond_bend_tors: only bonded atom, bend angle and torsional angle energies bond_bend_tors_onfo: bond, bend, torsional and one-four interactions all: all energies included
\prop_clos_sig{0.001}	Used in (post-propagation) stochastic closure minimization routine. The larger the value the more stochastic component involved in the chain closure algorithm [J. Comp. Biol. 17(8):993-1010 (2010)].
\prop_notors_sig_scale{1.0}	Independent molecules like water and ions do not have to satisfy the closure relation and can be propagated with larger steps for faster equilibration. This is the scaling factor used to increase their average step size. (Will be multiplied to \prop_trans_sig{}, \prop_rot_sig{}.)
\prop_closcompl_type{trans_rot}	Determines how a fragments complex is propagated. trans: only translational degree of freedom rot: only rotational degree of freedom trans_rot (default): both rotational and translational degrees of freedom are used
\random_seed{}	Random seed value for pseudo number generator. Use a large integer. Default general seed is defined in General Constructor.
\scale_mass{none}	Scaling of atomic masses. Only used in \prop_type{cart} . none (default): no scaling all: all atom masses scaled backbone: only backbone atoms scaled (except H)
\scale_mass_value{1}	Scaling factor for all atoms except H.
\scale_mass_value_H{}	Scaling factor for H atoms.

\sa_temp_first{}	Starting temperature in simulated annealing minimization run (samc). In K > 0.
\sa_temp_last{0.1}	Final temperature in simulated annealing minimization run (samc). In K > 0.
\sa_rate{0.9995}	Rate at which temperature decreases from \sa_temp_first{} to \sa_temp_last{} for samc minimization routine. Temperature decreases as $T_{i+1} =$ \sa_rate{}$\times T_i$ up till $T_{i+1} =$ \sa_temp_last{}.
\stsamc_type{}	Function used for stsamc run. trigonom: trigonometric sine function linear: triangle function
\stsamc_period{4000}	Period of stsamc function. In number of MC steps, ≥ 100.
\stsamc_ampl{800}	Amplitude of stsamc function. In K, > 0.
\stsamc_shift{}	Temperature shift used in \minimize_type{stsamc} minimization.
\prop_DNA_closcompl_typel{}	DNA base-pairing complex type. intra_level: Base-pairs are held stationary but bases are allowed to move inter_level: Base-pairs move as rigid bodies. Bases are now allowed to move within base-pair intra_inter_level (default): Base-pairing is preserved while both bases and base-pair are allowed to move
\cancel_res_inter_replace{}	Controls the removal of local non-bonded interactions for the specified topology declared by \inter_replace_database_file{}. off (default): no interactions are turned off neighbor: interactions within a residue/base and those between the residue/base and first neighbor residue/base are turned off. local: interactions within a residue/base are turned off.

\neighbor_list_skin{1}	Used with \inter_list{neighbor_list}. Distance in Å .
\lnk_list_skin{}	Used with \inter_list{lnk_list}. Distance in Å .
\rinter_exclude_length{100}	Intermolecular interactions between atoms initially apart by this distance (in Å) will not interact during the entire simulation.
\prop_regions_type{}	Defines how regions are propagated in hierarchical sampling. superimpose: In one MC iteration all regions are moved. onebyone: Only one (randomly chosen) regions is moved in one MC iteration.