System parameters

~sim_mol_def[] parameters for input file	
parameter	*meaning*
\mol_parm_file{}	Input file with molecular topology.
\bond_database_file{}	Input file containing parameters of the bond interactions.
\bend_database_file{}	Input file containing bend angle potential parameters.
\tors_database_file{}	Input file containing torsional angle potential parameters.
\onfo_database_file{}	Input file containing onefour potential parameters.
\inter_database_file{}	Input file containing inter-molecular interaction parameters.
\pos_init_file{}	Input pdb file of initial conformation.
\pos_out_file{}	Output pdb file (only final conformation is saved).
\atom_pos_file{}	Output trajectory file.
\epot_file{}	Output potential energy file.
\einter_file{}	Output intermolecular energy file.
\cgres_model{}	Type of coarse grained model to use off (default): Full atomic details used. KB_1pt: Knowledge-based 1 center per residue model. KB_3pt: Knowledge-based 3 center per residue model. (Mostly used for proteins.) KB_5pt: Knowledge-based 3 center per residue model. (Mostly used for RNA.) KB_UA: Knowledge-based united atom model. Go: Go model BNL: BNL model
\tors_pos_file{}	Output file of torsional angles.

\hessian_file{}	Output file with Hessian.
\eighess_file{}	Output file with eigenvalues of Hessian.
\eigvechess_file{}	Output file with eigenvectors of Hessian.
\neutralize{none}	Neutralize charges on molecule by scaling the classical charges of the two most electronegative atoms of a residue/base so that the total charge of the residue/base is zero. off (default): none nucl: nucleic acids prot: proteins all: all molecules
\ddd{none}	Dielectric model used off: None DDOS: The dielectric damping model as described in Rohs *et al.* in Biophysical Journal, 76, 2760 (1999). Formula is $\varepsilon(r) = D - \frac{(D-D_0)}{2}[(rS)^2 + 2rS + 2]\exp(-rS)$ ce: The analytical form of the distance dependent dielectric with $\varepsilon(r) = 78.3 - 77.3(r/2c)^e/(\sinh(r/2c))^e$ as defined by Wang *et al.* in Biophysical Journal, 83, 382 (2002).
\ddd_D{80}	Value for D as defined in the DDOS model. Non-negative real number.
\ddd_D0{4}	Value for D_0 as defined in the DDOS model. Non-negative real number.
\ddd_S{0.4}	Value for S as defined in the DDOS model. Non-negative real number.
\ddd_c{0.5}	Value for c as defined in the ce model. Non-negative real number.
\ddd_e{6}	Value for e as defined in the ce model. Non-negative real number.

\force_const_cutoff{off}	Controls intramolecular force constant. off (default): no control bond: only force constants related to bond stretches are affected. bond_bend: force constants related to bond stretches and bond angles are affected.
\force_const_cutoff_bond{}	Upper bound (in K/Å ^{2}) for force constants for bond stretches. In case a bond stretch has a force constant larger then specified here then the corresponding force constant is replaced by the specified one. Otherwise the force constant is not affected.
\force_const_cutoff_bend{}	Upper bound (in K/Å ^{2}) for force constants for bond angles. In case a bend stretch has a force constant larger then specified here then the corresponding force constant is replaced by the specified one. Otherwise the force constant is not affected.
\inter_replace_database_file{}	Specify topology to replace the internal energy potential with one declared by \inter_replace_database_file{}.
\inter_replace_type{}	Topology of \cancel_res_inter_replace{} type. E.g. KB_5pt, KB_UA.
\energy_term{}	Declares explicitly which energies to include or exclude. For instance, "inter" turns on the internal energy while "inter_off" turns it off. Can be used with "bond", "bend", "tors", "onfo", "inter", "cryo_em" and "constraint". By default all energies are included.
\cryo_em_database_file{}	Database file for cryo-EM data.
\cryo_em_expermnt_file{}	Experimental cryo-EM data.
\region_database_file{}	File specifying hierarchical move-sets.