AMBER20_DD_BOOST Documentation

The following table lists the keywords that are specific to AMBER20_DD_BOOST package. Brief descriptions are provided. For additional details refer to *AMBER20 Reference Manual*.

Variables	Entry	Description
scalpha	*real number*	The α parameter in equations 23.5 and 23.6 in AMBER20 Manual, its default value is 0.
scbeta	*real number*	The parameter β in equation 23.7 in AMBER20 Manual. Default value is 12 Å^2.
gti_add_sc	*int*	Flag to control the non-bonded interactions between the common and softcore regions, and within the softcore regions. 1: AMBER18 default 2: AMBER20 default 5: AMBER20 with torsion term scaled
gti_scale_beta	*int*	Flag to control *scbeta* behavior. 0: default, original *scbeta* behavior 1: *scbeta* is defined as unit-less and scaled by σ_{ij}
gti_cut	*int*	0: default in versions prior to AMBER20. 1: default, the non-bond cutoff, defined by *cutoff*, will not have effect on the internal softcore non-bonded terms.
gti_cut_sc_on	*real number*	Threshold distance for switching on of softcore smoothing. If undefined, *gti_cut_sc_on* is set to *cutoff* - 2 Å. Must be smaller than the value of *gti_cut_sc_off*.
gti_cut_sc_off	*real number*	Threshold distance for switching off of softcore smoothing. Must be smaller than or equal to the value of *cutoff*.
gti_lam_sch	*int*	Flag for λ-scheduling. 0: default, λ-scheduling is disabled. 1: λ-scheduling is enabled.
gti_ele_sc	*int*	Flag for the electrostatic softcore potentials 0: default when *gti_lam_sch*=0, smoothstep function is not utilized. 1: SSC(2) is utilized for electrostatic interactions
gti_vdw_sc	*int*	Flag for the vdW softcore potentials 0: default when *gti_lam_sch*=0, smoothstep function is not utilized. 1: SSC(2) is utilized for vdW interactions
gti_cut_sc	*int*	Flag to determine if tail smoothing will be applied to softcore potentials.

		0: default, no tail smoothing to SC 1: add smoothing to SC-vdW, beginning at *gti_cut_sc_on* and ending at *gti_cut_sc_off*; using SSC(2). 2: add smoothing to SC-vdW and SC-elec, beginning at *gti_cut_sc_on* and ending at *gti_cut_sc_off*.
gti_ele_exp	*int*	The exponent of $r_{elec,\,sc}$ (m) in the softcore function; the default value is 2.
gti_vdw_exp	*int*	The exponent of $r_{vdw,\,sc}$ (n) in the softcore function; the default value is 6.