**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*](https://ambermd.org/doc12/Amber20.pdf).

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| **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 Å2. |
| 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 σij |
| 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 relec, sc (m) in the softcore function; the default value is 2. |
| gti\_vdw\_exp | *int* | The exponent of rvdw, sc (n) in the softcore function; the default value is 6. |