

Table 1. Parameters of the contact and distance constraints.

Range /Å	DeepCDpred score (s)	Upper boundary	Lower boundary	Standard deviation	Weight
bin 0 - 8	≥ 0.9			0.5	2.5
	≥ 0.8 & < 0.9	$-10.8 * s + 16.7$	3.2	0.7	1.5
	< 0.8			1.0	1.0
bin 8 - 13	≥ 0.8	$-12 * s + 23.5$	7.5	1	1.5
	< 0.8			1.5	0.5
bin 13 - 18	≥ 0.8	$-8.6 * s + 25.17$	$8.6 * s + 4.84$	1.5	0.8
	< 0.8			1.0	0.3
bin 18 - 23	≥ 0.8	$-7.2 * s + 29.2$	$7.2 * s + 11.2$	1.5	0.6
	< 0.8			1.0	0.3