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Improved Parameters For The Martini Coarse-Grained Protein Force Field

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Supplementary information

Table 1: Mapping of the Amino Acids for the old (2.1) and new (2.2 and 2.2p) Martini force fields.

Side chain	CG representation			Mapping scheme[a]
	2.1	2.2	2.2p	
Leu	aC1[b]	aC1[b]	C1[b]	
Ile	aC1[b]	aC1[b]	C1[b]	
Val	aC2[b]	aC2[b]	C2[b]	
Pro	aC2[b]	C3	C3	
Met	C5	C5	C5	
Cys	C5	C5	C5	
Ser	P1	P1	N0-$(dN\text{-}dP)_{\pm 0.40}$	
Thr	P1	P1	N0-$(dN\text{-}dP)_{\pm 0.36}$	
Asn	P5	P5	Nda-$(dN\text{-}dP)_{\pm 0.46}$	
Gln	P4	P4	Nda-$(dN\text{-}dP)_{\pm 0.42}$	
Asp^S	Qa	Qa	Qa-dN_{-1}	
Asp (uncharged)	P3	P3	P3	
Glu^-	Qa	Qa	Qa-dN_{-1}	
Glu (uncharged)	P1	P1	P1	
Arg^+	N0-Qd	N0-Qd	N0-Qd-dP_{+1}	N0:Cβ-Cγ-Cδ-Nε
Arg (uncharged)	N0-P4	N0-P4	N0-P4	Qd/P4: Cξ-Nω1-Nω2
Lys^+	C3-Qd	C3-Qd	C3-Qd-dP_{+1}	C3: Cβ-Cγ-Cδ
Lys (uncharged)	C3-P1	C3-P1	C3-P1	Qd/P1:Cε-Nω
His	-	SC4-SP1-SQd	SC4-SP1-SQd-dP_{+1}	SC4:Cβ-Cγ
His (uncharged)	SC4-SP1-SP1	SC4-SP1-SP1	SC4-SP1-SP1	SP1/Qd: Cδ-Nε SP1/Qd: Nδ-Cε
Phe	SC4-SC4-SC4	SC5-SC5-SC5	SC5-SC5-SC5	SC5:Cβ-Cψ-Cδ1 SC5: Cδ2-Cε2 SC5: Cε1-Cξ
Tyr	SC4-SC4-SP1	SC4-SC4-SP1	SC4-SC4-SP1	SC4: Cβ-Cγ-Cδ1 SC4: Cδ2-Cε3 SP1: Cε1-Cξ-Oη
Trp	SC4-SP1-SC4-SC4	SC4-SNd-SC5-SC5	SC4-SNd-SC5-SC5	SC4: Cβ-Cγ-Cδ2 SNd: Cδ1-Nε-Cε1 SC4/5: Cε2-Cξ2 SC4/5: Cε1-Cω

[a] The mapping scheme is reported only for amino acid side chains consisting of more than one CG particle. (Partially) Charged dummy particles (dN or dP) or not considered in the mapping scheme. [b] For the C1 and C2 particle types of the amino acids in the non-polarizable forcefield (2.1 and 2.2), the interaction with the Q particles has been modified from the standard Martini forcefield. In order to avoid clashes between these particle pairs, in Martini 2.1 the Lennard-Jones parameter σ has been restored from 0.62 to the standard value of 0.47nm. The interactions were dubbed aC1 and aC2.

Table 2:Backbone Particle Type in Different Kinds of Secondary Structure[a,b]

	coil bend free	Helix	Helix (N-terminus/ C-terminus)	β-strand turn
backbone	P5	N0	Nd/Na	Nda
Gly	P5	N0	Nd/Na	Nda
Ala	P4	C5	N0	N0
Pro	P4	C5	N0/Na	N0

[a]These parameters have not been changed in Martini 2.2 with respect to Martini 2.1
[b]Both glycine and alanine have no side chain.

Table 3: Backbone Bonded Parameters used in Amino Acid Side Chains

	d_{BB} (nm)		K_{BB} (kJ nm^{-2} mol^{-1})		θ_{BBB} (deg)		K_{BBB} (kJ mol^{-1})		ψ_{BBB} (deg)		K_{BBBB} (kJ mol^{-1})	
Version	2.1	2.2	2.1	2.2	2.1	2.2	2.1	2.2	2.1	2.2	2.1	2.2
helix	0.35	0.31	1250	constraint	96[a]	96[a]	700	700	60	60	400	400
coil	0.35	0.35	200	1250	127	127	25	20				
extended	0.35	0.35	1250	1250	134	134	25	25	180	180	10	10
turn	0.35	0.35	500	1250	100	100	25	20				
bend	0.35	0.35	400	1250	130	130	25	20				

[a] $\theta_{BBB} = 98°$ when proline is in the helix; $K_{BBB} = 100$ kJ mol^{-1}

Table 4: Equilibrium Bond Length and Force Constant Used in Amino Acid Side Chains[a]

side chain	d (nm)	K (kJ nm^{-2} mol^{-1})
Leu	0.33	7500
Ile	0.31	constraint
Val	0.265	constraint
Pro	0.30	7500
Met	0.40	2500
Cys	0.31	7500
Ser	0.25	7500
Thr	0.26	constraint
Asn	0.32	5000
Gln	0.4	5000
Asp	0.32	7500
Glu	0.4	5000
Arg d_{BS}	0.33	5000
Arg d_{SS}	0.34	5000
Lys d_{BS}	0.33	5000
Lys d_{SS}	0.28	5000
His d_{BS}	0.32	7500
His d_{SS}	0.27	constraint
Phe d_{BS}	0.31	5000
Phe d_{SS}	0.27	constraint
Tyr d_{BS}	0.32	5000
Tyr d_{SS}	0.27	constraint
Trp d_{BS}	0.3	5000
Trp d_{SS}	0.27	constraint
Cys-Cys d_{S-S}	0.39	5000

[a]These parameters have not been changed in Martini 2.2 with respect to Martini 2.1

Table 5: Equilibrium Angles, Improper Dihedral Angles and Force Constants Used in Amino Acid Side Chains[a]

Side chain	θ (deg)	K (kJ mol^{-1})
θ_{BBS} (all)	100	25
θ_{BSS} (Lys, Arg)	180	25
θ_{BSS} (His, Tyr, Phe)	150	50
θ_{BSS} (Trp)	90, 210	50, 50
Side chain	**ψ (deg)**	**K (kJ rad^{-2} mol^{-1})**
ψ_{BSSS} (His, Tyr, Phe)	0	50
ψ_{BSSS} (Trp)	0,0	50, 200

[a]These parameters have not been changed in Martini 2.2 with respect to Martini 2.1

Table 6: Dummy bead bonded interactions for charged and polar side chains in the Martini 2.2p forcefield

Side chain	$d_{Q\text{-}D}/d_{D\text{-}D}$ (nm)	$K_{Q\text{-}D}/d_{D\text{-}D}$ (kJ nm^{-2} mol^{-1})
Charged (Arg, Lys, Glu, Asp, His)	0.11[a]	constraint
Polar (Gln, Asn, Ser, Thr)	0.28[b]	constraint

[a]The dummy bead is bound to the bead that maps the charged atom. [b] The dummy beads are bound to each other. The side chain bead is a virtual site positioned at the center of mass of the dummy beads. There are no bonds between the dummy beads and the virtual site.