

Table S1. Used energy parameters not included in the CHARMM force field. All used potentials are harmonical potentials. The energy E_i is given by $E_i = K_i(\zeta - \zeta_0)^2$, where K_i is the force constant, ζ is the value of the bond length, bond angle or improper angle and ζ_0 is the value around which the bonding term fluctuates, i. e the equilibrium point of the potential. The values are given either in Å or in grad, the force constants are given in kcal mol⁻¹ Å⁻² for the bond lengths and in kcal mol⁻¹ rad⁻² for the bond angles and the improper torsions.

energy term	force constant	value
	K_i	ζ_0
Bonds		
O H ₂ O – Pd	600.0	2.20
N _{ε2} His – Pd	600.0	2.01
N _{δ1} His – Pd	600.0	2.01
Bond Angles		
H H ₂ O – O H ₂ O – Pd	200.0	109.5
O H ₂ O – Pd – O H ₂ O	200.0	90.0
O H ₂ O – Pd – O H ₂ O	200.0	90.0
C _{ε1} His – N _{ε2} His – Pd	200.0	127.0
C _{δ2} His – N _{ε2} His – Pd	200.0	125.5
C _{ε1} His – N _{δ1} His – Pd	200.0	127.0
C _γ His – N _{δ1} His – Pd	200.0	125.5
Improper Torsions		
Pd – O H ₂ O – O H ₂ O – O H ₂ O	400.0	0.0
Pd – O H ₂ O – N _{δ1} – O H ₂ O	400.0	0.0
Pd – O H ₂ O – N _{ε2} – O H ₂ O	400.0	0.0
C _γ His – N _{δ1} His – C _{δ2} His – C _β His	100.0	0.0

Table S2. Charges used in the molecular dynamics simulation.

residue	atom	charge	
		$N_{\delta 1}$	$N_{e 2}$
Pd	Pd	1.360	1.360
His	C_{γ}	0.220	0.220
	$N_{\delta 1}$	-0.510	-0.350
	$H_{\delta 1}$	-	0.220
	$C_{\delta 2}$	-0.050	-0.050
	$H_{\delta 2}$	0.090	0.090
	$C_{e 1}$	0.500	0.500
	$H_{e 1}$	0.130	0.130
	$N_{e 2}$	-0.350	-0.510
	$H_{e 2}$	0.220	-
H ₂ O trans	O	-0.740	-0.740
	H	0.416	0.416
H ₂ O	O	-0.728	-0.728
	H	0.416	0.416