residue	atom	ε/kJ.mol^{-1}	σ/Å	q
	N	0.711280	3.25	-0.30
	H1	0.000000	0.00	0.33
	H2	0.000000	0.00	0.33
	H3	0.000000	0.00	0.33
	CA	0.276144	3.50	0.25
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
1	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.22
	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.70
	OE1	0.878640	2.96	-0.80
	OE2	0.878640	2.96	-0.80
	C	0.439320	3.75	0.50
	O	0.878640	2.96	-0.50
	N	0.711280	3.25	-0.50
	H	0.000000	0.00	0.30
	CA	0.276144	3.50	0.14
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.22
2–20	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.70
	OE1	0.878640	2.96	-0.80
	OE2	0.878640	2.96	-0.80
	C	0.439320	3.75	0.50
	O	0.878640	2.96	-0.50
	N	0.711280	3.25	-0.50
	H	0.000000	0.00	0.30
	CA	0.276144	3.50	0.04
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.22
21	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.70
	OE1	0.878640	2.96	-0.80
	OE2	0.878640	2.96	-0.80
	C	0.439320	3.75	0.70
	O1	0.878640	2.96	-0.80
	O2	0.878640	2.96	-0.80

Table 1: Lennard-Jones and partial atomic charges for Poly-L-Glutamate (PGA).

atom	ε/kJ.mol^{-1}	σ/Å	q
$Na^{+,1}$	6.724270	1.89744	1.00
$Na^{+,2}$	0.011598	3.33045	1.00
Cl^{-}	0.492830	4.41724	-1.00

Table 2: Lennard-Jones and partial atomic charges for $Na^{+,1}$, $Na^{+,2}$, and Cl^{-}.

atom	ε/kJ.mol^{-1}	σ/Å	q
OW	0.650194	3.16557	-0.8476
HW1	0.000000	0.00000	0.4238
HW2	0.000000	0.00000	0.4238

Table 3: Lennard-Jones and partial atomic charges for (SPC/E) water.

residue	atom	ε/kJ.mol^{-1}	σ/Å	q
	N	0.711280	3.25	-0.30
	H1	0.000000	0.00	0.33
	H2	0.000000	0.00	0.33
	H3	0.000000	0.00	0.33
	CA	0.276144	3.50	0.25
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
1	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.12
	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.52
	OE1	0.878640	2.96	-0.44
	OE2	0.711280	3.00	-0.53
	HE2	0.000000	0.00	0.45
	C	0.439320	3.75	0.50
	O	0.878640	2.96	-0.50
	N	0.711280	3.25	-0.50
	H	0.000000	0.00	0.30
	CA	0.276144	3.50	0.14
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.12
2–20	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.52
	OE1	0.878640	2.96	-0.44
	OE2	0.711280	3.00	-0.53
	HE2	0.000000	0.00	0.45
	C	0.439320	3.75	0.50
	O	0.878640	2.96	-0.50
	N	0.711280	3.25	-0.50
	H	0.000000	0.00	0.30
	CA	0.276144	3.50	0.04
	HA	0.125520	2.50	0.06
	CB	0.276144	3.50	-0.12
	HB1	0.125520	2.50	0.06
	HB2	0.125520	2.50	0.06
	CG	0.276144	3.50	-0.12
21	HG1	0.125520	2.50	0.06
	HG2	0.125520	2.50	0.06
	CD	0.439320	3.75	0.52
	OE1	0.878640	2.96	-0.44
	OE2	0.711280	3.00	-0.53
	HE2	0.000000	0.00	0.45
	C	0.439320	3.75	0.70
	O1	0.878640	2.96	-0.80
	O2	0.878640	2.96	-0.80

Table 4: Lennard-Jones and partial atomic charges for Poly-L-Glutamic acid (PGL).