

Partial atomic charges for the PNA backbone. Partial atomic charges for the atoms of the PNA backbone are listed in the table below.

atom name	atom type	partial atomic charge
C1'	C	0.51
O1'	O	-0.51
C2'	CT2	-0.16
H2'	HB	0.09
H2''	HB	0.09
N2'	NH3	-0.07
C5'	CT2	-0.16
H5'	HB	0.09
H5''	HB	0.09
C6'	CT2	0.08
H6'	HB	0.04
H6''	HB	0.04
N1'	NH1	-0.47
H1'	H	0.31
C3'	C	0.51
O3'	O	-0.51
C4'	CT2	-0.15
H4'	HB	0.09
H4''	HB	0.09

Force field parameters. Below we list the additional PNA parameters used in our simulations that are not provided in the standard CHARMM27 parameter files. The last column contains information about reference systems that the data are from.

Bonds:

CT2	NN2	400.0	1.460	CN8 - NN2
CT2	NN2B	400.0	1.458	CN8 - NN2B
NH3	C	370.0	1.3389	+/- 0.0091, 1PUP cryst. data, NH1 - C

Angles:

CN1	NN2	CT2	70.0	115.4	CN1 - NN2 - CN9
CN1T	NN2B	CT2	70.0	116.0	CN1T - NN2B - CN9
CN3	NN2	CT2	70.0	120.5	CN3 - NN2 - CN9
CN3	NN2B	CT2	70.0	122.0	CN3 - NN2B - CN9
CN4	NN2	CT2	70.0	127.8	CN4 - NN2 - CN9
CN4	NN2B	CT2	70.0	126.9	CN4 - NN2B - CN8
CN5	NN2	CT2	70.0	125.9	CN5 - NN2 - CN9
CN5	NN2B	CT2	70.0	125.9	CN5 - NN2B - CN8
CT2	NH3	C	50.0	122.0	+/- 2.2, 1PUP cryst. data, CT2 - NH1 - C
CT2	NH3	CT2	60.0	109.5	26.00 2.466 CTL2 - NTL - CTL2
HB	CT2	CT2	26.5	110.1	22.53 2.1790 HA - CT2 - CT2
NH3	C	CT2	80.0	118.6	+/- 1.5, 1PUP cryst. data, NH1 - C - CT2
NH3	CT2	HB	45.0	107.5	35.00 2.1010 NN6 - CN8 - HN8
NN2	CT2	HB	33.43	110.1	HN8 - CN8 - NN2
NN2B	CT2	HB	33.43	110.1	HN8 - CN8 - NN2B
NN2	CT2	C	43.7	109.3	+/- 1.2, 1PUP cryst. data, NH3 - CT2 - C
NN2B	CT2	C	43.7	109.3	+/- 1.2, 1PUP cryst. data, NH3 - CT2 - C
O	C	NH3	80.0	120.6	+/- 1.3, 1PUP cryst. data, O - C - NH1

Dihedrals:

CN1	NN2	CT2	C	0.19	3	0.0	CN5 - NN2B - CT2 - C
CN1	NN2	CT2	HB	0.19	3	0.0	CN1 - NN2 - CN9 - HN9
CN1T	NN2B	CT2	C	0.19	3	0.0	CN5 - NN2B - CT2 - C
CN1T	NN2B	CT2	HB	0.19	3	0.0	CN1T - NN2B - CN9 - HN9
CN3	NN2	CT2	C	0.00	3	0.0	CN4 - NN2B - CT2 - C
CN3	NN2	CT2	HB	0.00	3	0.0	CN3 - NN2 - CN9 - HN9
CN3	NN2B	CT2	C	0.00	3	0.0	CN4 - NN2B - CT2 - C
CN3	NN2B	CT2	HB	0.00	3	0.0	CN3 - NN2B - CN9 - HN9
CN4	NN2	CT2	C	0.00	3	0.0	CN4 - NN2B - CT2 - C
CN4	NN2	CT2	HB	0.00	3	0.0	CN4 - NN2 - CN9 - HN9
CN4	NN2B	CT2	C	0.00	3	0.0	CN4 - NN2B - CN8 - CN9
CN4	NN2B	CT2	HB	0.00	3	0.0	CN4 - NN2 - CN8 - HN8
CN5	NN2	CT2	C	0.19	3	0.0	CN5 - NN2B - CT2 - C
CN5	NN2	CT2	HB	0.19	3	0.0	CN5 - NN2 - CN9 - HN9
CN5	NN2B	CT2	C	0.19	3	0.0	CN5 - NN2B - CN8 - CN9
CN5	NN2B	CT2	HB	0.19	3	0.0	CN5 - NN2 - CN8 - HN8

CT2	NH3	C	CT2	1.40	2	180.0	(13)
CT2	NH3	C	O	1.40	2	180.0	(13)
H	NH1	CT2	CT2	0.00	1	0.0	H - NH1 - CT2 - CT3
NH2	CC	CT2	HB	0.00	3	180.0	NH2 - CC - CT2 - HA
X	CT2	C	X	0.05	6	180.0	X - CTL2 - CL - X

Improper:

NN2	CN1	CN3	CT2	90.00	0	0.00	CN2 - X - X - NN1
NN2B	CN1T	CN3	CT2	90.00	0	0.00	CN2 - X - X - NN1
NN2	CN4	CN5	CT2	90.00	0	0.00	CN2 - X - X - NN1
NN2B	CN4	CN5	CT2	90.00	0	0.00	CN2 - X - X - NN1
OC	X	X	CC	100.00	0	0.00	OBL - X - X - CL
NH3	CT1	CT2	C	90.00	0	0.00	CN2 - X - X - NN1
NH3	CT2	CT2	C	90.00	0	0.00	CN2 - X - X - NN1