Supporting Information (Model 2 Parameters) for: Accurate prediction of temperature-dependent phase behavior of disordered proteins

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Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
A	R	0.049480	0.089916	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	H	0.049480	0.027216	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	K	0.049480	0.019117	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	D	0.049480	0.079096	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	E	0.049480	0.085622	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	S	0.049480	0.061600	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	T	0.049480	0.030758	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	N	0.049480	0.193849	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	Q	0.049480	0.200448	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	C	0.049480	0.069311	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	G	0.049480	0.096470	-1.16417224e-04	5.42590026e-02	-8.46961697e+00	0.15	0	0	0	0
A	P	0.049480	0.078677	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	A	0.049480	0.049480	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
A	V	0.049480	0.005578	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
A	I	0.049480	0.000395	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
A	L	0.049480	0.010998	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
A	M	0.049480	0.039564	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
A	F	0.049480	0.391642	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	Y	0.049480	0.419186	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0
A	W	0.049480	0.550297	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70	0	0	0	0

TABLE I: Fitness function parameters for ε_{ij} where i = A in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
C	R	0.069311	0.089916	0	0	0	0	0	0	0	0
C	H	0.069311	0.027216	0	0	0	0	0	0	0	0
C	K	0.069311	0.019117	0	0	0	0	0	0	0	0
C	D	0.069311	0.079096	0	0	0	0	0	0	0	0
C	E	0.069311	0.085622	0	0	0	0	0	0	0	0
C	S	0.069311	0.061600	0	0	0	0	0	0	0	0
C	T	0.069311	0.030758	0	0	0	0	0	0	0	0
C	N	0.069311	0.193849	0	0	0	0	0	0	0	0
C	Q	0.069311	0.200448	0	0	0	0	0	0	0	0
C	C	0.069311	0.069311	0	0	0	0	0	0	0	0
C	G	0.069311	0.096470	0	0	0	0	0	0	0	0
C	P	0.069311	0.078677	0	0	0	0	0	0	0	0
C	A	0.069311	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
C	V	0.069311	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
C	I	0.069311	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
C	L	0.069311	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
C	M	0.069311	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
C	F	0.069311	0.391642	0	0	0	0	0	0	0	0
C	Y	0.069311	0.419186	0	0	0	0	0	0	0	0
C	W	0.069311	0.550297	0	0	0	0	0	0	0	0

TABLE II: Fitness function parameters for ε_{ij} where i = C in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
D	R	0.079096	0.089916	0	0	0	0	0	0	0	0
D	H	0.079096	0.027216	0	0	0	0	0	0	0	0
D	K	0.079096	0.019117	0	0	0	0	0	0	0	0
D	D	0.079096	0.079096	0	0	0	0	0	0	0	0
D	E	0.079096	0.085622	0	0	0	0	0	0	0	0
D	S	0.079096	0.061600	0	0	0	0	0	0	0	0
D	T	0.079096	0.030758	0	0	0	0	0	0	0	0
D	N	0.079096	0.193849	0	0	0	0	0	0	0	0
D	Q	0.079096	0.200448	0	0	0	0	0	0	0	0
D	C	0.079096	0.069311	0	0	0	0	0	0	0	0
D	G	0.079096	0.096470	0	0	0	0	0	0	0	0
D	P	0.079096	0.078677	0	0	0	0	0	0	0	0
D	A	0.079096	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
D	V	0.079096	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
D	I	0.079096	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
D	L	0.079096	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
D	M	0.079096	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
D	F	0.079096	0.391642	0	0	0	0	0	0	0	0
D	Y	0.079096	0.419186	0	0	0	0	0	0	0	0
D	W	0.079096	0.550297	0	0	0	0	0	0	0	0

TABLE III: Fitness function parameters for ε_{ij} where i = D in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
E	R	0.085622	0.089916	0	0	0	0	0	0	0	0
E	H	0.085622	0.027216	0	0	0	0	0	0	0	0
E	K	0.085622	0.019117	0	0	0	0	0	0	0	0
E	D	0.085622	0.079096	0	0	0	0	0	0	0	0
E	E	0.085622	0.085622	0	0	0	0	0	0	0	0
E	S	0.085622	0.061600	0	0	0	0	0	0	0	0
E	T	0.085622	0.030758	0	0	0	0	0	0	0	0
E	N	0.085622	0.193849	0	0	0	0	0	0	0	0
E	Q	0.085622	0.200448	0	0	0	0	0	0	0	0
E	C	0.085622	0.069311	0	0	0	0	0	0	0	0
E	G	0.085622	0.096470	0	0	0	0	0	0	0	0
E	P	0.085622	0.078677	0	0	0	0	0	0	0	0
E	A	0.085622	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
E	V	0.085622	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
E	I	0.085622	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
E	L	0.085622	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
E	M	0.085622	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
E	F	0.085622	0.391642	0	0	0	0	0	0	0	0
E	Y	0.085622	0.419186	0	0	0	0	0	0	0	0
E	W	0.085622	0.550297	0	0	0	0	0	0	0	0

TABLE IV: Fitness function parameters for ε_{ij} where i = E in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
F	R	0.391642	0.089916	0	0	0	0	0	0	0	0
F	H	0.391642	0.027216	0	0	0	0	0	0	0	0
F	K	0.391642	0.019117	0	0	0	0	0	0	0	0
F	D	0.391642	0.079096	0	0	0	0	0	0	0	0
F	E	0.391642	0.085622	0	0	0	0	0	0	0	0
F	S	0.391642	0.061600	0	0	0	0	0	0	0	0
F	T	0.391642	0.030758	0	0	0	0	0	0	0	0
F	N	0.391642	0.193849	0	0	0	0	0	0	0	0
F	Q	0.391642	0.200448	0	0	0	0	0	0	0	0
F	C	0.391642	0.069311	0	0	0	0	0	0	0	0
F	G	0.391642	0.096470	0	0	0	0	0	0	0	0
F	P	0.391642	0.078677	0	0	0	0	0	0	0	0
F	A	0.391642	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
F	V	0.391642	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
F	I	0.391642	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
F	L	0.391642	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
F	M	0.391642	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
F	F	0.391642	0.391642	0	0	0	0	0	0	0	0
F	Y	0.391642	0.419186	0	0	0	0	0	0	0	0
F	W	0.391642	0.550297	0	0	0	0	0	0	0	0

TABLE V: Fitness function parameters for ε_{ij} where i = F in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
G	R	0.096470	0.089916	0	0	0	0	0	0	0	0
G	H	0.096470	0.027216	0	0	0	0	0	0	0	0
G	K	0.096470	0.019117	0	0	0	0	0	0	0	0
G	D	0.096470	0.079096	0	0	0	0	0	0	0	0
G	E	0.096470	0.085622	0	0	0	0	0	0	0	0
G	S	0.096470	0.061600	0	0	0	0	0	0	0	0
G	T	0.096470	0.030758	0	0	0	0	0	0	0	0
G	N	0.096470	0.193849	0	0	0	0	0	0	0	0
G	Q	0.096470	0.200448	0	0	0	0	0	0	0	0
G	C	0.096470	0.069311	0	0	0	0	0	0	0	0
G	G	0.096470	0.096470	0	0	0	0	0	0	0	0
G	P	0.096470	0.078677	0	0	0	0	0	0	0	0
G	A	0.096470	0.049480	0	0	0	0	-1.16417224e-04	5.42590026e-02	-8.46961697e+00	0.15
G	V	0.096470	0.005578	0	0	0	0	-2.24644855e-04	1.15406051e-01	-1.92322375e+01	0.20
G	I	0.096470	0.000395	0	0	0	0	-2.11751849e-04	1.10797972e-01	-1.85218569e+01	0.20
G	L	0.096470	0.010998	0	0	0	0	-2.29222797e-04	1.17281979e-01	-1.91871215e+01	0.20
G	M	0.096470	0.039564	0	0	0	0	-1.37150154e-04	8.01341277e-02	-1.76908670e+01	0.20
G	F	0.096470	0.391642	0	0	0	0	0	0	0	0
G	Y	0.096470	0.419186	0	0	0	0	0	0	0	0
G	W	0.096470	0.550297	0	0	0	0	0	0	0	0

TABLE VI: Fitness function parameters for ε_{ij} where i = G in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
H	R	0.027216	0.089916	0	0	0	0	0	0	0	0
H	H	0.027216	0.027216	0	0	0	0	0	0	0	0
H	K	0.027216	0.019117	0	0	0	0	0	0	0	0
H	D	0.027216	0.079096	0	0	0	0	0	0	0	0
H	E	0.027216	0.085622	0	0	0	0	0	0	0	0
H	S	0.027216	0.061600	0	0	0	0	0	0	0	0
H	T	0.027216	0.030758	0	0	0	0	0	0	0	0
H	N	0.027216	0.193849	0	0	0	0	0	0	0	0
H	Q	0.027216	0.200448	0	0	0	0	0	0	0	0
H	C	0.027216	0.069311	0	0	0	0	0	0	0	0
H	G	0.027216	0.096470	0	0	0	0	0	0	0	0
H	P	0.027216	0.078677	0	0	0	0	0	0	0	0
H	A	0.027216	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
H	V	0.027216	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
H	I	0.027216	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
H	L	0.027216	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
H	M	0.027216	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
H	F	0.027216	0.391642	0	0	0	0	0	0	0	0
H	Y	0.027216	0.419186	0	0	0	0	0	0	0	0
H	W	0.027216	0.550297	0	0	0	0	0	0	0	0

TABLE VII: Fitness function parameters for ε_{ij} where i = H in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
I	R	0.000395	0.089916	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	H	0.000395	0.027216	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	K	0.000395	0.019117	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	D	0.000395	0.079096	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	E	0.000395	0.085622	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	S	0.000395	0.061600	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	T	0.000395	0.030758	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	N	0.000395	0.193849	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	Q	0.000395	0.200448	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	C	0.000395	0.069311	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	G	0.000395	0.096470	-1.48226294e-04	1.10797972e-01	-1.85218569e+01	0.20	0	0	0	0
I	P	0.000395	0.078677	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	A	0.000395	0.049480	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
I	V	0.000395	0.005578	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
I	I	0.000395	0.000395	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
I	L	0.000395	0.010998	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
I	M	0.000395	0.039564	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
I	F	0.000395	0.391642	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	Y	0.000395	0.419186	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0
I	W	0.000395	0.550297	-9.88175293e-05	1.10797972e-01	-1.85218569e+01	0.70	0	0	0	0

TABLE VIII: Fitness function parameters for ε_{ij} where i = I in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
K	R	0.019117	0.089916	0	0	0	0	0	0	0	0
K	H	0.019117	0.027216	0	0	0	0	0	0	0	0
K	K	0.019117	0.019117	0	0	0	0	0	0	0	0
K	D	0.019117	0.079096	0	0	0	0	0	0	0	0
K	E	0.019117	0.085622	0	0	0	0	0	0	0	0
K	S	0.019117	0.061600	0	0	0	0	0	0	0	0
K	T	0.019117	0.030758	0	0	0	0	0	0	0	0
K	N	0.019117	0.193849	0	0	0	0	0	0	0	0
K	Q	0.019117	0.200448	0	0	0	0	0	0	0	0
K	C	0.019117	0.069311	0	0	0	0	0	0	0	0
K	G	0.019117	0.096470	0	0	0	0	0	0	0	0
K	P	0.019117	0.078677	0	0	0	0	0	0	0	0
K	A	0.019117	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
K	V	0.019117	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
K	I	0.019117	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
K	L	0.019117	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
K	M	0.019117	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
K	F	0.019117	0.391642	0	0	0	0	0	0	0	0
K	Y	0.019117	0.419186	0	0	0	0	0	0	0	0
K	W	0.019117	0.550297	0	0	0	0	0	0	0	0

TABLE IX: Fitness function parameters for ε_{ij} where i = K in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
L	R	0.010998	0.089916	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	H	0.010998	0.027216	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	K	0.010998	0.019117	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	D	0.010998	0.079096	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	E	0.010998	0.085622	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	S	0.010998	0.061600	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	T	0.010998	0.030758	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	N	0.010998	0.193849	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	Q	0.010998	0.200448	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	C	0.010998	0.069311	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	G	0.010998	0.096470	-1.60455958e-04	1.17281979e-01	-1.91871215e+01	0.20	0	0	0	0
L	P	0.010998	0.078677	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	A	0.010998	0.049480	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
L	V	0.010998	0.005578	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
L	I	0.010998	0.000395	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
L	L	0.010998	0.010998	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
L	M	0.010998	0.039564	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
L	F	0.010998	0.391642	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	Y	0.010998	0.419186	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0
L	W	0.010998	0.550297	-1.06970639e-04	1.17281979e-01	-1.91871215e+01	0.70	0	0	0	0

TABLE X: Fitness function parameters for ε_{ij} where i = L in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
M	R	0.039564	0.089916	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	H	0.039564	0.027216	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	K	0.039564	0.019117	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	D	0.039564	0.079096	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	E	0.039564	0.085622	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	S	0.039564	0.061600	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	T	0.039564	0.030758	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	N	0.039564	0.193849	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	Q	0.039564	0.200448	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	C	0.039564	0.069311	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	G	0.039564	0.096470	-1.37150154e-04	8.01341277e-02	-1.76908670e+01	0.20	0	0	0	0
M	P	0.039564	0.078677	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	A	0.039564	0.049480	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
M	V	0.039564	0.005578	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
M	I	0.039564	0.000395	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
M	L	0.039564	0.010998	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
M	M	0.039564	0.039564	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
M	F	0.039564	0.391642	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	Y	0.039564	0.419186	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0
M	W	0.039564	0.550297	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70	0	0	0	0

TABLE XI: Fitness function parameters for ε_{ij} where i = M in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
N	R	0.193849	0.089916	0	0	0	0	0	0	0	0
N	H	0.193849	0.027216	0	0	0	0	0	0	0	0
N	K	0.193849	0.019117	0	0	0	0	0	0	0	0
N	D	0.193849	0.079096	0	0	0	0	0	0	0	0
N	E	0.193849	0.085622	0	0	0	0	0	0	0	0
N	S	0.193849	0.061600	0	0	0	0	0	0	0	0
N	T	0.193849	0.030758	0	0	0	0	0	0	0	0
N	N	0.193849	0.193849	0	0	0	0	0	0	0	0
N	Q	0.193849	0.200448	0	0	0	0	0	0	0	0
N	C	0.193849	0.069311	0	0	0	0	0	0	0	0
N	G	0.193849	0.096470	0	0	0	0	0	0	0	0
N	P	0.193849	0.078677	0	0	0	0	0	0	0	0
N	A	0.193849	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
N	V	0.193849	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
N	I	0.193849	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
N	L	0.193849	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
N	M	0.193849	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
N	F	0.193849	0.391642	0	0	0	0	0	0	0	0
N	Y	0.193849	0.419186	0	0	0	0	0	0	0	0
N	W	0.193849	0.550297	0	0	0	0	0	0	0	0

TABLE XII: Fitness function parameters for ε_{ij} where i = N in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
P	R	0.078677	0.089916	0	0	0	0	0	0	0	0
P	H	0.078677	0.027216	0	0	0	0	0	0	0	0
P	K	0.078677	0.019117	0	0	0	0	0	0	0	0
P	D	0.078677	0.079096	0	0	0	0	0	0	0	0
P	E	0.078677	0.085622	0	0	0	0	0	0	0	0
P	S	0.078677	0.061600	0	0	0	0	0	0	0	0
P	T	0.078677	0.030758	0	0	0	0	0	0	0	0
P	N	0.078677	0.193849	0	0	0	0	0	0	0	0
P	Q	0.078677	0.200448	0	0	0	0	0	0	0	0
P	C	0.078677	0.069311	0	0	0	0	0	0	0	0
P	G	0.078677	0.096470	0	0	0	0	0	0	0	0
P	P	0.078677	0.078677	0	0	0	0	0	0	0	0
P	A	0.078677	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
P	V	0.078677	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
P	I	0.078677	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
P	L	0.078677	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
P	M	0.078677	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
P	F	0.078677	0.391642	0	0	0	0	0	0	0	0
P	Y	0.078677	0.419186	0	0	0	0	0	0	0	0
P	W	0.078677	0.550297	0	0	0	0	0	0	0	0

TABLE XIII: Fitness function parameters for ε_{ij} where i = P in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
Q	R	0.200448	0.089916	0	0	0	0	0	0	0	0
Q	H	0.200448	0.027216	0	0	0	0	0	0	0	0
Q	K	0.200448	0.019117	0	0	0	0	0	0	0	0
Q	D	0.200448	0.079096	0	0	0	0	0	0	0	0
Q	E	0.200448	0.085622	0	0	0	0	0	0	0	0
Q	S	0.200448	0.061600	0	0	0	0	0	0	0	0
Q	T	0.200448	0.030758	0	0	0	0	0	0	0	0
Q	N	0.200448	0.193849	0	0	0	0	0	0	0	0
Q	Q	0.200448	0.200448	0	0	0	0	0	0	0	0
Q	C	0.200448	0.069311	0	0	0	0	0	0	0	0
Q	G	0.200448	0.096470	0	0	0	0	0	0	0	0
Q	P	0.200448	0.078677	0	0	0	0	0	0	0	0
Q	A	0.200448	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
Q	V	0.200448	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
Q	I	0.200448	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
Q	L	0.200448	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
Q	M	0.200448	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
Q	F	0.200448	0.391642	0	0	0	0	0	0	0	0
Q	Y	0.200448	0.419186	0	0	0	0	0	0	0	0
Q	W	0.200448	0.550297	0	0	0	0	0	0	0	0

TABLE XIV: Fitness function parameters for ε_{ij} where i = Q in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
R	R	0.089916	0.089916	0	0	0	0	0	0	0	0
R	H	0.089916	0.027216	0	0	0	0	0	0	0	0
R	K	0.089916	0.019117	0	0	0	0	0	0	0	0
R	D	0.089916	0.079096	0	0	0	0	0	0	0	0
R	E	0.089916	0.085622	0	0	0	0	0	0	0	0
R	S	0.089916	0.061600	0	0	0	0	0	0	0	0
R	T	0.089916	0.030758	0	0	0	0	0	0	0	0
R	N	0.089916	0.193849	0	0	0	0	0	0	0	0
R	Q	0.089916	0.200448	0	0	0	0	0	0	0	0
R	C	0.089916	0.069311	0	0	0	0	0	0	0	0
R	G	0.089916	0.096470	0	0	0	0	0	0	0	0
R	P	0.089916	0.078677	0	0	0	0	0	0	0	0
R	A	0.089916	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
R	V	0.089916	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
R	I	0.089916	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
R	L	0.089916	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
R	M	0.089916	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
R	F	0.089916	0.391642	0	0	0	0	0	0	0	0
R	Y	0.089916	0.419186	0	0	0	0	0	0	0	0
R	W	0.089916	0.550297	0	0	0	0	0	0	0	0

TABLE XV: Fitness function parameters for ε_{ij} where i = R in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
S	R	0.061600	0.089916	0	0	0	0	0	0	0	0
S	H	0.061600	0.027216	0	0	0	0	0	0	0	0
S	K	0.061600	0.019117	0	0	0	0	0	0	0	0
S	D	0.061600	0.079096	0	0	0	0	0	0	0	0
S	E	0.061600	0.085622	0	0	0	0	0	0	0	0
S	S	0.061600	0.061600	0	0	0	0	0	0	0	0
S	T	0.061600	0.030758	0	0	0	0	0	0	0	0
S	N	0.061600	0.193849	0	0	0	0	0	0	0	0
S	Q	0.061600	0.200448	0	0	0	0	0	0	0	0
S	C	0.061600	0.069311	0	0	0	0	0	0	0	0
S	G	0.061600	0.096470	0	0	0	0	0	0	0	0
S	P	0.061600	0.078677	0	0	0	0	0	0	0	0
S	A	0.061600	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
S	V	0.061600	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
S	I	0.061600	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
S	L	0.061600	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
S	M	0.061600	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
S	F	0.061600	0.391642	0	0	0	0	0	0	0	0
S	Y	0.061600	0.419186	0	0	0	0	0	0	0	0
S	W	0.061600	0.550297	0	0	0	0	0	0	0	0

TABLE XVI: Fitness function parameters for ε_{ij} where i = S in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
T	R	0.030758	0.089916	0	0	0	0	0	0	0	0
T	H	0.030758	0.027216	0	0	0	0	0	0	0	0
T	K	0.030758	0.019117	0	0	0	0	0	0	0	0
T	D	0.030758	0.079096	0	0	0	0	0	0	0	0
T	E	0.030758	0.085622	0	0	0	0	0	0	0	0
T	S	0.030758	0.061600	0	0	0	0	0	0	0	0
T	T	0.030758	0.030758	0	0	0	0	0	0	0	0
T	N	0.030758	0.193849	0	0	0	0	0	0	0	0
T	Q	0.030758	0.200448	0	0	0	0	0	0	0	0
T	C	0.030758	0.069311	0	0	0	0	0	0	0	0
T	G	0.030758	0.096470	0	0	0	0	0	0	0	0
T	P	0.030758	0.078677	0	0	0	0	0	0	0	0
T	A	0.030758	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
T	V	0.030758	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
T	I	0.030758	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
T	L	0.030758	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
T	M	0.030758	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
T	F	0.030758	0.391642	0	0	0	0	0	0	0	0
T	Y	0.030758	0.419186	0	0	0	0	0	0	0	0
T	W	0.030758	0.550297	0	0	0	0	0	0	0	0

TABLE XVII: Fitness function parameters for ε_{ij} where i = T in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
V	R	0.005578	0.089916	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	H	0.005578	0.027216	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	K	0.005578	0.019117	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	D	0.005578	0.079096	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	E	0.005578	0.085622	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	S	0.005578	0.061600	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	T	0.005578	0.030758	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	N	0.005578	0.193849	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	Q	0.005578	0.200448	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	C	0.005578	0.069311	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	G	0.005578	0.096470	-2.24644855e-04	1.15406051e-01	-1.92322375e+01	0.20	0	0	0	0
V	P	0.005578	0.078677	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	A	0.005578	0.049480	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
V	V	0.005578	0.005578	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
V	I	0.005578	0.000395	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
V	L	0.005578	0.010998	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
V	M	0.005578	0.039564	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
V	F	0.005578	0.391642	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	Y	0.005578	0.419186	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0
V	W	0.005578	0.550297	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70	0	0	0	0

TABLE XVIII: Fitness function parameters for ε_{ij} where i = V in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
W	R	0.550297	0.089916	0	0	0	0	0	0	0	0
W	H	0.550297	0.027216	0	0	0	0	0	0	0	0
W	K	0.550297	0.019117	0	0	0	0	0	0	0	0
W	D	0.550297	0.079096	0	0	0	0	0	0	0	0
W	E	0.550297	0.085622	0	0	0	0	0	0	0	0
W	S	0.550297	0.061600	0	0	0	0	0	0	0	0
W	T	0.550297	0.030758	0	0	0	0	0	0	0	0
W	N	0.550297	0.193849	0	0	0	0	0	0	0	0
W	Q	0.550297	0.200448	0	0	0	0	0	0	0	0
W	C	0.550297	0.069311	0	0	0	0	0	0	0	0
W	G	0.550297	0.096470	0	0	0	0	0	0	0	0
W	P	0.550297	0.078677	0	0	0	0	0	0	0	0
W	A	0.550297	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
W	V	0.550297	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
W	I	0.550297	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
W	L	0.550297	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
W	M	0.550297	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
W	F	0.550297	0.391642	0	0	0	0	0	0	0	0
W	Y	0.550297	0.419186	0	0	0	0	0	0	0	0
W	W	0.550297	0.550297	0	0	0	0	0	0	0	0

TABLE XIX: Fitness function parameters for ε_{ij} where i = W in Mpipi-T Model 2

Amino Acid i	Amino Acid j	$\varepsilon_{ii,\mathrm{Mpipi}}$	$\varepsilon_{jj,\mathrm{Mpipi}}$	a_i	b_i	c_i	α_i	a_j	b_j	c_j	α_j
Y	R	0.419186	0.089916	0	0	0	0	0	0	0	0
Y	H	0.419186	0.027216	0	0	0	0	0	0	0	0
Y	K	0.419186	0.019117	0	0	0	0	0	0	0	0
Y	D	0.419186	0.079096	0	0	0	0	0	0	0	0
Y	E	0.419186	0.085622	0	0	0	0	0	0	0	0
Y	S	0.419186	0.061600	0	0	0	0	0	0	0	0
Y	T	0.419186	0.030758	0	0	0	0	0	0	0	0
Y	N	0.419186	0.193849	0	0	0	0	0	0	0	0
Y	Q	0.419186	0.200448	0	0	0	0	0	0	0	0
Y	C	0.419186	0.069311	0	0	0	0	0	0	0	0
Y	G	0.419186	0.096470	0	0	0	0	0	0	0	0
Y	P	0.419186	0.078677	0	0	0	0	0	0	0	0
Y	A	0.419186	0.049480	0	0	0	0	-6.84807201e-05	5.42590026e-02	-8.46961697e+00	0.70
Y	V	0.419186	0.005578	0	0	0	0	-1.49763237e-04	1.15406051e-01	-1.92322375e+01	0.70
Y	I	0.419186	0.000395	0	0	0	0	-1.41167899e-04	1.10797972e-01	-1.85218569e+01	0.70
Y	L	0.419186	0.010998	0	0	0	0	-1.52815198e-04	1.17281979e-01	-1.91871215e+01	0.70
Y	M	0.419186	0.039564	0	0	0	0	-9.14334357e-05	8.01341277e-02	-1.76908670e+01	0.70
Y	F	0.419186	0.391642	0	0	0	0	0	0	0	0
Y	Y	0.419186	0.419186	0	0	0	0	0	0	0	0
Y	W	0.419186	0.550297	0	0	0	0	0	0	0	0

TABLE XX: Fitness function parameters for ε_{ij} where i = Y in Mpipi-T Model 2