Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S5. List of all relative interaction free energy scales, interaction propensity scales and contact coefficients derived in this study.

Sidechain analog relative free energy for different nitrogenous bases

	DMP	PYR^{u}	PYR^{u*}	PUR^{u}	PUR^{u*}
ala	-6.54	-2.07	-2.24	-3.52	-3.24
arg	1.21	-1.64	-1.38	0.57	-1.09
asn	-1.34	-3.23	-3.46	-2.96	-3.82
asp	2.20	-2.58	-2.84	-0.39	-1.48
cys	-4.90	-3.34	-3.70	-5.48	-4.70
gln	-1.91	-3.03	-3.29	-3.56	-3.79
glu	1.20	-2.98	-2.97	-0.92	-1.98
gly	-	-	-	-	-
his	-0.51	-2.06	-2.05	-2.44	-2.60
ile	-8.52	-2.35	-2.44	-5.35	-4.05
leu	-8.61	-2.41	-2.43	-5.00	-3.85
lys	-0.50	-1.74	-1.34	-0.17	-0.99
met	-5.06	-2.86	-3.37	-5.36	-4.45
phe	-7.60	-2.45	-3.02	-5.39	-4.61
pro	-	-	-	-	-
ser	-0.27	-2.01	-2.00	-1.20	-2.06
thr	-1.55	-1.87	-1.97	-2.25	-2.27
trp	-4.85	-5.77	-6.07	-5.74	-5.04
tyr	-3.73	-2.49	-2.83	-5.24	-4.20
val	-8.02	-2.16	-2.53	-4.66	-3.90

*sidechain analog interaction propensities derived from mixed systems,

where both PURu and PYRu molecules were present at the same time

Sidechain analog interaction propensity scales for different nitrogenous bases

	DMP	SEM_{DMP_sca}	PYR^{u}	SEM_{PYRu_sca}	PYR^{u*}	SEM_{PYRu*_sca}	PUR^{u}	SEM_{PURu_sca}	PUR^{u*}	SEM_{PURu*_sca}
ala	-11.96	0.06	0.24	0.05	3.24	0.04	-5.75	0.09	1.72	0.06
arg	85.46	0.26	12.84	0.38	48.50	0.34	70.03	0.29	61.85	0.29
asn	66.14	0.31	25.43	0.38	37.39	0.38	29.60	0.41	42.75	0.36
asp	265.08	0.35	89.66	0.55	123.55	0.60	178.90	0.63	147.34	0.61
cys	-14.93	0.17	-0.45	0.16	7.00	0.15	-24.21	0.19	3.20	0.16
gln	59.92	0.32	24.66	0.39	38.55	0.38	13.59	0.43	42.56	0.37
glu	259.35	0.36	82.98	0.54	121.20	0.59	162.16	0.67	142.63	0.60
gly	-	-	-	-	-	-	-	-	-	-
his	81.43	0.28	42.30	0.34	62.44	0.32	36.20	0.39	61.70	0.33
ile	-36.88	0.09	-1.06	0.09	6.72	0.09	-31.31	0.17	-1.32	0.14
leu	-35.90	0.09	-1.10	0.09	7.16	0.09	-28.08	0.17	0.58	0.13
lys	110.91	0.28	38.58	0.49	80.44	0.42	103.67	0.30	97.02	0.36
met	-24.51	0.18	2.59	0.16	11.71	0.15	-35.76	0.22	2.77	0.20
phe	-50.09	0.13	-4.93	0.14	4.95	0.14	-48.23	0.20	-6.59	0.19
pro	-	-	-	-	-	-	-	-	-	-
ser	56.30	0.24	34.68	0.28	43.96	0.28	40.92	0.30	45.50	0.27
thr	47.35	0.26	34.00	0.28	43.30	0.28	28.72	0.33	44.42	0.28
trp	-34.77	0.28	-12.93	0.26	4.85	0.25	-70.86	0.30	-7.09	0.30
tyr	19.12	0.27	26.01	0.31	38.13	0.31	-33.60	0.39	28.42	0.33
val	-29.08	0.08	0.33	0.07	5.47	0.08	-20.83	0.15	-0.05	0.12

*sidechain analog interaction propensities derived from mixed systems,

where both PURu and PYRu molecules were present at the same time

Sidechain analog contact coefficient scales for different nitrogenous bases

	DMP	PYR^{u}	PYR^{u*}	PUR^{u}	PUR^{u*}	PUR^{u}:PYR^{u*}
ala	2.59	0.64	0.66	0.88	0.78	1.19
arg	0.07	0.88	0.78	0.22	0.44	0.56
asn	0.29	1.13	1.28	0.79	1.04	0.81
asp	0.05	1.02	1.13	0.28	0.47	0.42
cys	1.49	1.03	1.17	2.21	1.49	1.27
gln	0.34	1.11	1.27	1.03	1.07	0.84
glu	0.07	1.04	1.12	0.35	0.53	0.47
gly	-	-	-	-	-	-
his	0.23	0.69	0.66	0.70	0.74	1.13
ile	6.58	0.83	0.86	2.02	1.22	1.41
leu	7.07	0.82	0.84	1.81	1.10	1.31
lys	0.06	0.89	0.70	0.14	0.22	0.31
met	1.44	0.84	0.96	1.88	1.31	1.37
phe	5.65	0.94	1.17	2.65	1.83	1.57
pro	-	-	-	-	-	-
ser	0.16	0.64	0.62	0.37	0.49	0.79
thr	0.22	0.64	0.65	0.54	0.52	0.80
trp	1.93	1.21	1.52	3.07	2.18	1.43
tyr	0.85	0.86	1.00	2.02	1.37	1.37
val	5.37	0.75	0.85	1.50	1.12	1.32

*sidechain analog contact coefficients derived from mixed systems,

where both PURu and PYRu molecules were present at the same time

Amino acid relative free energy for different nitrogenous bases

	DMP	PYR^{u}	PYR^{u*}	PUR^{u}	PUR^{u*}
ala	3.16	-3.60	-3.65	-0.06	-2.23
arg	5.12	-2.14	-1.79	1.10	0.07
asn	2.94	-3.36	-3.35	-1.77	-2.90
asp	5.45	-3.19	-3.32	-0.08	-2.00
cys	1.32	-3.28	-3.49	-1.06	-2.62
gln	2.27	-2.77	-3.16	-0.76	-2.73
glu	4.92	-2.81	-3.06	-0.16	-1.47
gly	4.57	-3.54	-3.88	-1.05	-2.73
his	2.28	-2.82	-2.96	-1.53	-2.91
ile	0.38	-3.04	-3.36	-1.26	-2.13
leu	0.05	-3.02	-3.09	-1.30	-2.03
lys	5.50	-2.47	-1.98	1.09	-0.84
met	0.46	-2.81	-3.19	-1.91	-3.17
phe	-0.61	-3.18	-3.53	-2.47	-3.77
pro	1.50	-2.86	-3.22	-1.36	-2.71
ser	3.89	-3.28	-3.43	-0.42	-2.48
thr	2.20	-3.37	-3.44	-1.66	-2.51
trp	-1.14	-4.42	-5.01	-3.69	-3.94
tyr	0.27	-2.84	-2.98	-2.71	-3.38
val	0.91	-3.13	-2.97	-1.17	-1.36

*amino acid relative free energies derived from mixed systems,

where both PURu and PYRu molecules were present at the same time

Amino acid interaction propensity scales for different nitrogenous bases

	DMP	SEM_{DMP_aa}	PYR^{u}	SEM_{PYRu_aa}	PYR^{u*}	SEM_{PYRu*_aa}	PUR^{u}	SEM_{PURu_aa}	PUR^{u*}	SEM_{PURu*_aa}
ala	279.47	0.41	56.25	0.66	108.97	0.70	205.55	0.69	148.13	0.66
arg	381.31	0.45	75.17	0.74	174.87	0.74	267.11	0.76	232.27	0.69
asn	341.22	0.54	44.35	0.77	113.14	0.85	153.22	0.99	154.74	0.82
asp	506.78	0.55	94.27	0.85	174.85	0.96	327.24	1.03	243.80	0.93
cys	270.04	0.47	39.39	0.66	89.99	0.72	170.68	0.71	134.15	0.69
gln	358.16	0.53	73.30	0.77	117.29	0.83	219.32	0.91	167.62	0.79
glu	546.18	0.64	124.51	0.89	210.38	0.96	342.71	1.25	284.32	0.94
gly	288.63	0.40	55.51	0.68	96.82	0.75	178.37	0.81	137.52	0.72
his	324.31	0.54	63.44	0.73	119.44	0.78	163.77	0.86	153.49	0.77
ile	257.62	0.43	56.03	0.64	101.25	0.70	157.51	0.76	143.27	0.67
leu	249.47	0.43	49.99	0.65	103.86	0.66	155.00	0.77	146.65	0.64
lys	416.27	0.47	79.47	0.86	195.39	0.85	308.76	0.76	252.84	0.78
met	256.19	0.47	46.30	0.66	86.93	0.78	122.04	0.80	114.97	0.78
phe	242.00	0.44	31.70	0.68	82.62	0.70	130.90	0.71	116.18	0.69
pro	244.33	0.40	65.67	0.57	96.62	0.63	136.73	0.71	119.20	0.63
ser	300.66	0.46	56.27	0.70	105.15	0.76	194.94	0.76	145.51	0.73
thr	281.06	0.48	47.38	0.66	100.30	0.73	139.59	0.86	140.26	0.71
trp	257.45	0.48	15.71	0.68	79.52	0.73	93.55	0.76	121.00	0.72
tyr	317.55	0.48	63.89	0.71	126.13	0.78	125.26	0.87	168.09	0.74
val	262.27	0.42	61.70	0.65	124.25	0.68	160.08	0.69	163.20	0.65

*amino acid interaction propensities derived from mixed systems,

where both PURu and PYRu molecules were present at the same time

Amino acid contact coefficient scales for different nitrogenous bases

	DMP	PYR^{u}	PYR^{u*}	PUR^{u}	PUR^{u*}	PUR^{u}:PYR^{u*}
ala	0.03	1.48	1.52	0.22	0.51	0.34
arg	0.02	1.10	0.97	0.21	0.32	0.33
asn	0.07	1.74	1.75	0.62	0.90	0.52
asp	0.02	1.72	1.81	0.33	0.58	0.32
cys	0.09	1.64	1.84	0.43	0.75	0.41
gln	0.08	1.45	1.81	0.42	0.86	0.48
glu	0.02	1.48	1.57	0.32	0.51	0.32
gly	0.02	1.52	1.73	0.31	0.62	0.36
his	0.09	1.25	1.39	0.56	0.89	0.64
ile	0.07	1.44	1.64	0.38	0.55	0.33
leu	0.09	1.49	1.65	0.40	0.53	0.32
lys	0.01	1.37	1.11	0.17	0.30	0.27
met	0.09	1.49	1.82	0.57	0.90	0.49
phe	0.36	1.41	1.78	0.83	1.32	0.74
pro	0.05	1.15	1.38	0.39	0.67	0.49
ser	0.03	1.52	1.66	0.31	0.65	0.39
thr	0.06	1.60	1.66	0.54	0.67	0.41
trp	0.36	1.61	1.93	1.22	1.36	0.70
tyr	0.18	1.31	1.44	0.81	0.85	0.59
val	0.06	1.37	1.32	0.37	0.40	0.30

*amino acid contact coefficients derived from mixed systems,

where both PURu and PYRu molecules were present at the same time