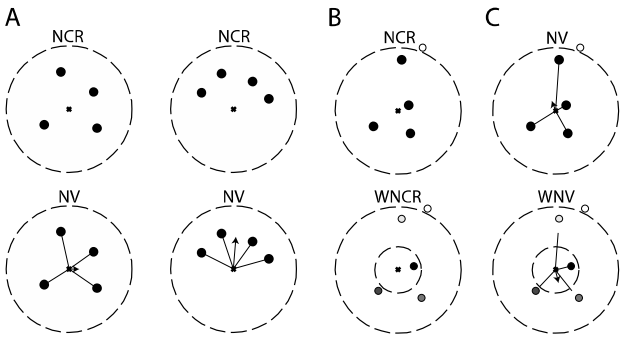
	0.00–0.05	0.05–0.10	0.10–0.15	0.15–0.20	0.20–0.25	0.25–0.30	0.30–0.35	0.35–0.40	0.40–0.45	0.45–0.50	0.50–0.55	0.55–0.60	0.60–0.65	0.65–0.70	0.70–0.75	0.75–0.80	0.80–0.85	0.85–0.90	0.90–0.95	0.95–1.00
A	-0.42	-1.42	-1.05	-0.60	-0.38	-0.08	-0.01	0.14	0.10	-0.04	0.06	0.40	0.26	0.85	1.34	2.19	2.93	3.88	4.23	5.35
R	1.90	0.14	-0.44	-0.57	-0.63	-0.63	-0.72	-0.70	-0.68	-0.67	-0.38	0.05	0.33	0.86	1.73	2.34	3.26	4.39	4.31	7.61
N	0.77	-0.49	-0.51	-0.40	-0.33	-0.39	-0.39	-0.42	-0.45	-0.55	-0.44	-0.20	-0.12	0.20	0.60	1.41	3.11	4.49	5.64	6.04
D	1.56	0.05	-0.28	-0.31	-0.29	-0.28	-0.41	-0.46	-0.55	-0.71	-0.59	-0.35	-0.36	0.02	0.44	1.25	2.54	4.20	4.92	7.06
C	-0.66	-1.66	-1.44	-0.94	-0.67	-0.16	0.11	0.43	0.74	1.12	1.37	2.22	2.43	3.10	3.45	3.88	5.59	6.28	4.49	6.28
Q	1.17	-0.24	-0.43	-0.41	-0.41	-0.43	-0.41	-0.53	-0.67	-0.74	-0.57	-0.13	-0.01	0.53	1.09	1.91	2.93	3.98	4.75	6.62
E	1.99	0.45	0.03	-0.04	-0.12	-0.27	-0.33	-0.45	-0.66	-0.89	-0.77	-0.47	-0.52	-0.03	0.45	1.36	2.66	3.96	4.40	6.51
G	0.24	-1.00	-0.89	-0.54	-0.28	-0.17	-0.08	-0.09	-0.10	-0.26	-0.26	-0.25	-0.02	0.09	0.63	2.04	3.45	3.83	4.43	5.35
H	0.75	-0.59	-0.99	-0.90	-0.79	-0.58	-0.52	-0.38	-0.26	-0.14	0.08	0.37	0.62	1.02	1.40	2.11	3.07	3.68	4.17	5.43
I	-0.49	-1.64	-1.43	-0.91	-0.52	-0.22	0.05	0.29	0.53	0.70	1.03	1.57	2.21	2.65	3.04	3.98	5.08	5.32	5.42	7.03
L	-0.22	-1.50	-1.43	-0.98	-0.63	-0.35	-0.12	0.19	0.39	0.60	0.96	1.57	1.77	2.47	2.73	3.75	4.49	5.14	5.62	7.08
K	2.73	0.97	0.26	-0.03	-0.24	-0.46	-0.61	-0.68	-0.78	-0.84	-0.78	-0.39	-0.28	0.26	0.77	1.44	2.51	3.99	4.42	5.67
M	-0.14	-1.47	-1.30	-0.87	-0.64	-0.26	-0.07	0.00	0.19	0.37	0.65	1.06	1.36	1.62	2.13	2.35	3.10	3.17	3.59	5.20
F	-0.03	-1.48	-1.51	-1.09	-0.71	-0.38	-0.03	0.28	0.59	0.81	1.23	1.66	2.11	2.44	3.06	3.79	4.43	4.74	5.77	6.28
P	0.67	-0.55	-0.66	-0.51	-0.31	-0.26	-0.29	-0.29	-0.26	-0.36	-0.28	-0.35	-0.24	0.08	0.34	1.22	2.25	3.75	4.18	5.31
S	0.15	-0.90	-0.71	-0.46	-0.36	-0.32	-0.21	-0.20	-0.28	-0.38	-0.37	-0.13	0.01	0.42	0.82	1.52	2.55	3.70	4.00	5.54
T	0.26	-0.95	-0.78	-0.59	-0.47	-0.38	-0.34	-0.35	-0.36	-0.37	-0.31	0.03	0.33	0.93	1.36	2.29	3.23	3.96	4.33	6.31
W	0.42	-1.16	-1.48	-1.20	-0.87	-0.52	-0.29	0.18	0.36	0.52	1.09	1.62	1.71	2.47	3.00	3.52	4.10	4.91	6.30	5.20
Y	0.37	-1.17	-1.41	-1.16	-0.86	-0.61	-0.30	0.04	0.37	0.59	0.88	1.46	1.67	2.26	2.92	3.47	4.53	5.29	5.63	7.24
V	-0.60	-1.65	-1.29	-0.75	-0.44	-0.23	0.00	0.21	0.30	0.39	0.69	1.35	1.69	2.13	2.68	3.53	4.59	4.56	5.76	6.35

Supplementary Figure 1: The knowledge based potential used in the NV environment KBP, colored by value.

Supplementary Figure 1 shows the knowledge based potential use by the NV environment KBP. In practice, it is rare to see neighbor vector values of less then 0.05 or greater than 0.70, so unusually positive scores in this region of the knowledge based potential are artifacts due to low count numbers, and do not effect the behavior of the energy function in practice.



Supplementary Figure 2: (A) The left and right panels both have the same ROSETTA neighbor count (4) but very different degrees of burial. The neighbor vector method is able to distinguish between these cases by calculating the vectors between the query residue and its neighbors. The length of the vector indicates the degree of burial, with shorter vectors representing more buried residues. (B) The weighted NCR (WNCR) method gives a higher weight to neighbors near the query residue, smoothing the effect of small changes in composition on the measured degree of burial. (C) The combination of the NV and WNCR methods results in a more accurate measure

of residue distribution. In all panels, dotted lines represent lower and upper bounds for counts, the X marks the query residue, and circles represent residues surrounding the query residue.

Supplementary Figure 2 shows a schematic Representation of the ROSETTA Neighbor Count (NCR) and Neighbor Vector (NV) approximations of Solvent Accessible Surface Area, demonstrating cases where the NV method provides a more accurate assessment of solvent exposure.