

SUPPLEMENTAL TABLE 1. POSITIONAL SEQUENCE VARIABILITY SCORE<sup>a</sup>

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
Amino acid	I	F	L	V	M	W	C	Y	A	H	G	T	P	S	R	N	Q	E	D	K	I,L,V	Consensus	Index	Max (N)	Total (P)	Var	N Var	Totals
1	0	0	0	0	0	1	5999	3	0	0	0	0	0	2	5	0	0	0	0	0	0	C		5999	6010	0.18%	0.31%	
2	787	4	5	77	40	0	0	1	71	0	0	4901	9	85	3	2	1	17	0	7	869	T		4901	6010	18.45%	30.95%	
3	4	0	0	0	0	0	0	0	0	0	7	9	0	7	5971	0	0	0	0	12	4	R		5971	6010	0.65%	1.09%	
4	4	9	35	8	0	0	0	2	2	17	0	15	5906	10	2	0	0	0	0	0	47	P		5906	6010	1.73%	2.90%	
5	8	39	1	2	0	0	0	72	26	72	850	22	2	973	1	3923	3	0	13	3	11	N		3923	6010	34.73%	58.25%	
6	13	0	0	0	0	0	0	17	0	6	6	27	0	25	7	5838	3	10	29	29	13	N		5838	6010	2.86%	4.80%	Stem
7	17	2	0	0	0	0	0	43	1	11	0	23	2	10	2	5856	0	0	7	36	17	N		5856	6010	2.56%	4.30%	19.91%
8	84	0	3	11	4	0	0	0	7	0	0	5810	4	2	26	1	6	4	0	48	98	T	303	5810	6010	3.33%	5.58%	
9	62	2	3	2	6	0	0	1	5	0	22	9	1	79	5739	3	6	7	0	63	67	R	304	5739	6010	4.51%	7.56%	Hydrophilic
10	14	0	0	4	2	2	0	0	1	2	10	936	3	5	631	15	168	191	2	4024	18	K	305	4024	6010	33.04%	55.43%	65.78%
11	3	0	0	1	0	1	0	0	1	5	805	2	1	4896	250	13	6	1	10	15	4	S	306	4896	6010	18.54%	31.09%	
12	4434	8	37	1043	379	5	0	8	4	4	2	66	0	4	11	1	1	2	0	1	5514	I	307	5514	6010	8.25%	13.84%	Hydrophobic
13	16	2	3	0	3	2	1	45	20	1853	73	531	438	252	2427	283	53	0	0	8	19	R	308	2427	6010	59.62%	100.00%	15.55%
14	4998	89	412	61	395	0	0	1	3	14	0	20	2	6	4	0	1	0	0	4	5471	I	309	5471	6010	8.97%	15.04%	
15	23	0	1	4	0	0	0	0	86	1	5862	2	0	5	19	0	6	0	0	1	28	G	312	5862	6010	2.46%	4.13%	Turn
16	0	9	38	0	2	44	0	0	4	0	27	4	5823	8	3	0	48	0	0	0	38	P	313	5823	6010	3.11%	5.22%	20.40%
17	0	2	4	3	1	4	1	0	0	0	5945	0	17	0	21	0	6	4	0	2	7	G	314	5945	6010	1.08%	1.81%	
18	3	0	3	0	1	0	0	4	14	31	98	4	5	94	2069	0	3486	4	0	194	6	Q	315	3486	6010	42.00%	70.44%	
19	31	0	3	740	9	0	0	6	3173	1	1	1913	1	76	27	2	11	6	0	10	774	A	316	3173	6010	47.20%	79.18%	
20	110	5263	219	75	14	248	0	45	21	1	0	3	1	7	2	0	0	1	0	0	404	F	317	5263	6010	12.43%	20.85%	
21	13	277	13	20	1	5	4	5563	1	90	0	1	0	4	11	3	1	0	3	0	46	Y	318	5563	6010	7.44%	12.48%	
22	7	2	3	14	1	0	1	26	4116	5	21	1247	5	15	479	0	10	3	0	55	24	A	319	4116	6010	31.51%	52.86%	
23	38	0	2	3	26	0	0	1	149	17	1	5613	13	30	74	27	4	3	0	9	43	T	320	5613	6010	6.61%	11.08%	
24	1	0	0	0	0	0	0	2	4	6	5342	44	0	11	65	160	1	151	143	80	1	G		5342	6010	11.11%	18.64%	
25	6	0	3	10	4	0	0	5	434	12	317	29	5	52	150	121	368	1360	2960	174	19	D		2960	6010	50.75%	85.12%	
26	5523	0	7	443	9	0	0	1	1	0	3	12	1	1	3	0	1	1	1	3	5973	I		5973	6010	0.62%	1.03%	
27	5391	2	14	180	13	0	0	1	4	0	5	357	1	6	6	4	5	4	0	17	5585	I		5585	6010	7.07%	11.86%	
28	0	0	0	1	0	1	0	0	0	0	5948	2	0	2	27	1	0	18	1	9	1	G		5948	6010	1.03%	1.73%	
29	5	2	0	5	0	0	0	3	3	3	16	9	1	8	3	922	4	34	4967	25	10	D		4967	6010	17.35%	29.11%	
30	5898	0	10	27	10	0	0	1	0	0	0	28	24	0	2	5	0	0	1	4	5935	I		5935	6010	2.09%	2.09%	
31	6	0	1	0	0	0	0	0	0	0	13	8	0	9	5898	0	0	2	0	73	7	R		5898	6010	1.86%	3.13%	
32	4	0	16	0	0	2	0	3	21	23	2	2	2	10	210	12	4336	114	4	1249	20	Q		4336	6010	27.85%	46.72%	
33	0	0	0	5	0	0	0	0	5980	0	2	8	7	7	0	0	1	0	0	0	5	A		5980	6010	0.50%	0.84%	
34	1	56	3	0	0	1	3	1542	1	4333	0	0	3	14	11	9	28	0	5	0	4	H		4333	6010	27.90%	46.80%	
35	0	0	0	0	0	0	5996	4	0	0	2	0	0	4	4	0	0	0	0	0	0	C		5996	6010	0.23%	0.39%	

<sup>a</sup>Columns B–U count the total number of times a given amino acid occurs at that V3 position in the group of 6010 sequences used to create this table. Column V contains the sum of columns B, D, and E. Column X (Index) indicates the amino acid index number assigned in the PDB (index numbers are shown only for the loop crown region). Columns Y and Z are used in calculating the variability (*n* and *p*; see Materials and Methods). Column Z contains the value of the highest occurring amino acid (or acids, if column V contains the maximum) from the row. The nonnormalized positional variability score (column AA) is calculated using the equation  $1 - (n/p)$ . The normalized positional variability score (column AB) is calculated by multiplying column AA by a coefficient that fixes the most variable position at 100%. In this table the most variable position is found at the amino acid index number 308, and the resulting coefficient ~ 1.67.