Auxiliary material for "How effective for fold recognition is a potential of mean force that includes relative orientations between contacting residues in proteins?"

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TABLE I: Dependencies of the performance of fold recognition on the resolution of the orientational potential; dependencies on polar or Euler angles.

(A) Dependencies on polar angles

		$l_e^{max} = k_e^{max} = 0$, $\beta = 0.2$, $O_{cutoff} = \infty$							
l_p^{max}	c_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
4	0.0	23	-2.79	-2.09	-1.41	29	-2.66	-1.88	-1.45
	0.025	22	-2.77	-2.02	-1.41	28	-2.67	-1.82	-1.45
	0.050	23	-2.76	-2.08	-1.39	28	-2.70	-1.87	-1.49
5	0.0	31	-3.35	-2.57	-1.84	31	-2.68	-1.96	-1.46
	0.025	31	-3.37	-2.57	-1.84	30	-2.66	-1.93	-1.45
	0.050	30	-3.34	-2.54	-1.83	34	-2.72	-2.12	-1.47
6	0.0	27	-3.23	-2.55	-1.77	34	-2.69	-2.19	-1.45
	0.025	28	-3.24	-2.58	-1.76	34	-2.68	-2.16	-1.44
	0.050	29	-3.19	-2.63	-1.74	35	-2.72	-2.22	-1.47
7	0.0	30	-3.45	-2.60	-1.98	45	-2.93	-2.52	-1.57
	0.025	31	-3.46	-2.60	-1.98	45	-2.94	-2.53	-1.58
	0.050	30	-3.36	-2.60	-1.92	44	-2.89	-2.44	-1.57
8	0.0	28	-3.37	-2.59	-1.91	38	-2.73	-2.24	-1.48
	0.025	27	-3.36	-2.55	-1.89	39	-2.74	-2.27	-1.49
	0.050	30	-3.33	-2.71	-1.85	35	-2.71	-2.02	-1.50
9	0.0	25	-3.38	-2.43	-1.92	32	-2.66	-2.06	-1.54
	0.025	24	-3.36	-2.44	-1.90	33	-2.68	-2.08	-1.56
	0.050	29	-3.35	-2.56	-1.85	39	-2.71	-2.30	-1.58
10	0.0	27	-3.32	-2.55	-1.83	37	-2.55	-2.13	-1.52
	0.025	26	-3.31	-2.49	-1.82	36	-2.52	-2.14	-1.55
	0.050	27	-3.23	-2.46	-1.78	38	-2.59	-2.16	-1.59
11	0.0	28	-3.44	-2.67	-1.94	39	-2.68	-2.16	-1.71
	0.025	30	-3.48	-2.82	-1.92	39	-2.67	-2.18	-1.72
	0.050	28	-3.42	-2.66	-1.88	44	-2.77	-2.38	-1.80
12	0.0	25	-3.29	-2.45	-1.78	41	-2.70	-2.29	-1.76
	0.025	24	-3.30	-2.50	-1.77	40	-2.70	-2.29	-1.77
	0.050	25	-3.23	-2.52	-1.73	41	-2.71	-2.34	-1.79
13	0.0	30	-3.39	-2.73	-1.80	39	-2.80	-2.19	-1.83
	0.025	29	-3.38	-2.73	-1.80	40	-2.80	-2.20	-1.83
	0.050	25	-3.30	-2.49	-1.74	42	-2.76	-2.32	-1.86
14	0.0	31	-3.42	-2.89	-1.84	46	-2.87	-2.48	-1.91
	0.025	30	-3.44	-2.82	-1.82	47	-2.89	-2.53	-1.89
	0.050	28	-3.39	-2.77	-1.78	43	-2.82	-2.42	-1.90

(B) Dependencies on Euler angles

l_e^{max}		$l_p^{max} = 0$, $\beta = 0.2$, $O_{cutoff} = \infty$							
k_e^{max}	c_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
4	0.0	25	-3.18	-2.68	-1.78	33	-2.63	-2.26	-1.31
	0.025	25	-3.14	-2.71	-1.75	33	-2.61	-2.31	-1.29
	0.050	24	-3.13	-2.74	-1.73	24	-2.45	-1.94	-1.27
5	0.0	25	-3.26	-2.79	-1.77	44	-2.85	-2.55	-1.65
	0.025	26	-3.23	-2.80	-1.74	44	-2.84	-2.58	-1.61
	0.050	24	-3.16	-2.70	-1.70	34	-2.65	-2.24	-1.49
6	0.0	26	-3.25	-2.79	-1.83	47	-3.04	-2.78	-1.84
	0.025	24	-3.20	-2.57	-1.81	45	-3.00	-2.79	-1.77
	0.050	21	-3.13	-2.41	-1.76	42	-2.88	-2.61	-1.68
7	0.0	30	-3.31	-2.84	-1.88	52	-3.03	-2.94	-1.82
	0.025	28	-3.24	-2.70	-1.83	52	-3.02	-2.92	-1.73
	0.050	25	-3.18	-2.51	-1.75	47	-2.88	-2.77	-1.60

TABLE II: Dependencies of the performance of fold recognition on the resolution of the orientational potential; interdependencies between polar and Euler angles: Dependencies on l^{max} and cutoff O_{cutoff}.

		$l_e^{max} = k_e^{max} = l_p^{max}$, $\beta = 0.2$, $c_{cutoff} = 0.0$							
l_p^{max}	O_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
5	637	36	-3.80	-3.28	-2.25	52	-3.10	-2.86	-1.76
	960	35	-3.81	-3.33	-2.27	55	-3.17	-2.96	-1.83
	1792	38	-3.88	-3.30	-2.34	56	-3.23	-2.93	-1.96
6	64	27	-3.50	-2.90	-1.92	29	-2.63	-2.02	-1.47
	225	33	-3.70	-3.09	-2.11	42	-2.86	-2.66	-1.54
	637	36	-3.86	-3.21	-2.32	56	-3.20	-2.98	-1.87
	960	34	-3.80	-3.24	-2.32	60	-3.26	-3.25	-1.95
	1792	37	-3.87	-3.35	-2.40	60	-3.28	-3.14	-2.01
7	64	27	-3.53	-2.94	-1.93	32	-2.70	-2.06	-1.49
	225	31	-3.68	-3.04	-2.10	42	-2.86	-2.60	-1.53
	960	34	-3.82	-3.11	-2.33	59	-3.25	-3.17	-1.96
	1792	39	-3.92	-3.27	-2.43	55	-3.20	-3.05	-2.05

		$l_e^{max} = k_e^{max} = l_p^{max}$, $\beta = 0.2$, $c_{cutoff} = 0.025$							
l_p^{max}	O_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
4	960	34	-3.72	-3.24	-2.18	47	-2.97	-2.81	-1.59
	1584	37	-3.75	-3.29	-2.20	46	-3.00	-2.70	-1.64
	1792	36	-3.77	-3.27	-2.21	47	-3.01	-2.79	-1.67
5	637	35	-3.78	-3.29	-2.23	53	-3.10	-2.93	-1.74
	960	36	-3.82	-3.38	-2.27	56	-3.18	-3.02	-1.81
	1584	37	-3.85	-3.25	-2.32	55	-3.21	-2.91	-1.93
	1792	38	-3.87	-3.22	-2.33	55	-3.23	-2.92	-1.96
	2025	37	-3.87	-3.27	-2.36	56	-3.23	-2.96	-1.95
6	64	27	-3.50	-2.90	-1.91	28	-2.59	-1.98	-1.44
	225	29	-3.65	-3.00	-2.10	41	-2.84	-2.67	-1.51
	637	37	-3.86	-3.31	-2.32	55	-3.15	-3.04	-1.83
	960	37	-3.83	-3.33	-2.32	60	-3.24	-3.23	-1.92
	1584	38	-3.87	-3.34	-2.38	58	-3.23	-3.08	-1.98
	1792	37	-3.88	-3.22	-2.38	59	-3.27	-3.11	-2.00
	2025	38	-3.85	-3.25	-2.36	56	-3.21	-3.05	-1.99
7	64	27	-3.53	-2.95	-1.93	30	-2.63	-2.04	-1.46
	225	29	-3.65	-3.01	-2.10	43	-2.85	-2.64	-1.51
	637	37	-3.90	-3.31	-2.37	51	-3.12	-2.90	-1.85
	960	36	-3.85	-3.22	-2.34	57	-3.22	-3.11	-1.93
	1584	36	-3.88	-3.35	-2.38	54	-3.14	-3.00	-1.96
	1792	38	-3.91	-3.31	-2.42	53	-3.20	-2.94	-2.02
	2025	37	-3.87	-3.29	-2.40	54	-3.20	-3.02	-2.04

		$l_e^{max} = k_e^{max} = l_p^{max}$, $\beta = 0.2$, $c_{cutoff} = 0.05$							
l_p^{max}	O_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
5	960	35	-3.79	-3.18	-2.24	55	-3.15	-2.96	-1.74
	1792	36	-3.84	-3.28	-2.29	52	-3.16	-2.90	-1.86
6	960	33	-3.77	-2.99	-2.27	56	-3.19	-3.12	-1.82
	1792	35	-3.85	-3.19	-2.36	56	-3.21	-3.09	-1.89
7	960	33	-3.76	-2.98	-2.29	58	-3.21	-3.21	-1.85
	1792	35	-3.87	-3.12	-2.38	53	-3.18	-2.95	-1.91

TABLE III: Dependencies of the performance of fold recognition on the resolution of the orientational potential; interdependencies between polar and Euler angles: Dependencies on cutoff c_{cutoff}.

		$l_e^{max} = k_e^{max} = l_p^{max}$, $\beta = 0.2$, $O_{cutoff} = 960$							
l_p^{max}	c_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
5	0.0	35	-3.81	-3.33	-2.27	55	-3.17	-2.96	-1.83
	0.025	36	-3.82	-3.38	-2.27	56	-3.18	-3.02	-1.81
	0.050	35	-3.79	-3.18	-2.24	55	-3.15	-2.96	-1.74
6	0.0	34	-3.80	-3.24	-2.32	60	-3.26	-3.25	-1.95
	0.025	37	-3.83	-3.33	-2.32	60	-3.24	-3.23	-1.92
	0.050	33	-3.77	-2.99	-2.27	56	-3.19	-3.12	-1.82
7	0.0	34	-3.82	-3.11	-2.33	59	-3.25	-3.17	-1.96
	0.025	36	-3.85	-3.22	-2.34	57	-3.22	-3.11	-1.93
	0.050	33	-3.76	-2.98	-2.29	58	-3.21	-3.21	-1.85

		$l_e^{max} = k_e^{max} = l_p^{max}$, $\beta = 0.2$, $O_{cutoff} = 1792$							
l_p^{max}	c_{cutoff}	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
5	0.0	38	-3.88	-3.30	-2.34	56	-3.23	-2.93	-1.96
	0.025	38	-3.87	-3.22	-2.33	55	-3.23	-2.92	-1.96
	0.050	36	-3.84	-3.28	-2.29	52	-3.16	-2.90	-1.86
6	0.0	37	-3.87	-3.35	-2.40	60	-3.28	-3.14	-2.01
	0.025	37	-3.88	-3.22	-2.38	59	-3.27	-3.11	-2.00
	0.050	35	-3.85	-3.19	-2.36	56	-3.21	-3.09	-1.89
7	0.0	39	-3.92	-3.27	-2.43	55	-3.20	-3.05	-2.05
	0.025	38	-3.91	-3.31	-2.42	53	-3.20	-2.94	-2.02
	0.050	35	-3.87	-3.12	-2.38	53	-3.18	-2.95	-1.91

TABLE IV: Dependencies of the performance of fold recognition on the resolution of the orientational potential; interdependencies between polar and Euler angles: Dependencies on a parameter for small sample correction, β.

		$l_p^{max} = l_e^{max} = k_e^{max} = 6$, $c_{cutoff} = 0.025$							
O_{cutoff}	β	79 monomeric decoy sets				81 Ig decoy sets			
		#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$	#tops	$\overline{\log P_e}$	$\overline{\log P_r}$	$\overline{Z_e}$
960	0.1	35	-3.82	-3.26	-2.32	60	-3.25	-3.23	-1.93
	0.2	37	-3.83	-3.33	-2.32	60	-3.24	-3.23	-1.92
	0.5	35	-3.80	-3.24	-2.30	58	-3.23	-3.20	-1.91
	1	34	-3.78	-3.23	-2.28	58	-3.22	-3.19	-1.89
1584	0.1	38	-3.87	-3.34	-2.38	58	-3.23	-3.08	-1.97
	0.2	38	-3.87	-3.34	-2.38	58	-3.23	-3.08	-1.98
	0.5	38	-3.86	-3.32	-2.36	59	-3.24	-3.14	-1.97
	1	34	-3.82	-3.23	-2.34	56	-3.20	-3.02	-1.95
1792	0.1	36	-3.86	-3.15	-2.39	59	-3.27	-3.11	-2.00
	0.2	37	-3.88	-3.22	-2.38	59	-3.27	-3.11	-2.00
	0.5	36	-3.86	-3.22	-2.37	60	-3.27	-3.15	-1.99
	1	36	-3.85	-3.18	-2.34	57	-3.24	-3.05	-1.97
2025	0.2	38	-3.85	-3.25	-2.36	56	-3.21	-3.05	-1.99

TABLE V: The performance of scoring functions for each set of monomeric protein decoys.

Decoy set		The present potential, $e^c_{rr} + \Delta e^c + e^o + e^s$								BF[a]				TE-13[b]		SA[c]			Onizuka[d]	
	#decoys	rank$_e$	log P_e	Z_e	RMSD	rank$_r$	log P_r	Z_r	R^e	rank$_e$	Z_e	RMSD	R^e	rank$_e$	Z_e	rank$_e$	Z_e	R^e	rank$_e$	Z_e
4state_reduced																				
1 1CTF	631	1	-6.45	-4.11	0.00	1	-6.45	-2.97	0.70	1	-2.9	1.97	0.63	1	-4.20	1	-2.9	0.74	1	-3.37
2 1R69	676	1	-6.52	-4.28	0.00	1	-6.52	-3.10	0.69	11	-2.0	2.48	0.59	1	-4.06	1	-2.4	0.78	1	-4.30
3 1SN3	661	1	-6.49	-5.24	0.00	1	-6.49	-3.43	0.58	5	-2.7	1.31	0.40	6	-2.70	1	-3.3	0.45	1	-3.06
4 2CRO	675	1	-6.51	-4.10	0.00	1	-6.51	-2.80	0.66	22	-1.7	3.82	0.42	1	-3.48	1	-2.5	0.72	1	-2.97
5 3ICB	654	1	-6.48	-2.66	0.00	1	-6.48	-2.65	0.80	55	-1.4	1.92	0.76			22	-1.7	0.82	1	-2.81
6 4PTI	688	1	-6.53	-5.71	0.00	1	-6.53	-3.55	0.59	13	-2.0	1.49	0.29	7	-2.43	1	-3.3	0.60	1	-3.28
7 4RXN	678	1	-6.52	-4.99	0.00	1	-6.52	-3.27	0.60	2	-3.4	2.08	0.52	16	-1.97	1	-2.6	0.59	1	-4.05
fisa																				
8 1FC2	501	501	0.00	3.53	4.41	280	-0.58	-0.33	0.25					16	-1.67				371	0.37
9 1HDD-C	501	12	-3.73	-1.78	4.65	116	-1.46	-0.82	0.51					1	-4.35				47	-1.32
10 2CRO	501	1	-6.22	-5.13	0.00	1	-6.22	-4.39	0.12					1	-4.00				1	-2.46
11 4ICB	501	1	-6.22	-6.84	0.00	1	-6.22	-3.93	0.15											
fisa_casp3																				
12 1BG8-A	1201	17	-4.26	-2.07	11.88	832	-0.37	0.47	0.05					3	-2.98				6	-2.57
13 1BL0	972	39	-3.22	-1.74	7.07	120	-2.09	-1.38	0.28					3	-2.80				702	0.54
14 1EH2	2414	15	-5.08	-2.39	7.87	410	-1.77	-1.05	0.31					1	-6.04					
15 1JWE	1408	1	-7.25	-4.45	0.00	1	-7.25	-8.38	0.02										1	-2.91
16 SMD3	1201	1	-7.09	-7.39	0.00	1	-7.09	-8.07	0.16											
hg_structal																				
17 1ASH	30	1	-3.40	-4.58	0.00	1	-3.40	-3.41	0.73											
18 1BAB-B	30	1	-3.40	-2.38	0.00	1	-3.40	-1.73	0.93											
19 1COL-A	30	1	-3.40	-8.80	0.00	1	-3.40	-4.78	0.21											
20 1CPC-A	30	1	-3.40	-7.67	0.00	1	-3.40	-5.59	0.37											
21 1ECD	30	1	-3.40	-3.06	0.00	1	-3.40	-2.50	0.80											
22 1EMY	30	1	-3.40	-2.69	0.00	1	-3.40	-1.75	0.88											
23 1FLP	30	1	-3.40	-4.80	0.00	1	-3.40	-2.21	0.58											
24 1GDM	30	1	-3.40	-3.62	0.00	1	-3.40	-3.04	0.74											
25 1HBG	30	1	-3.40	-5.05	0.00	1	-3.40	-2.59	0.80											
26 1HBH-A	30	1	-3.40	-1.87	0.00	1	-3.40	-1.70	0.97											
27 1HBH-B	30	1	-3.40	-1.90	0.00	1	-3.40	-1.77	0.94											
28 1HDA-A	30	1	-3.40	-2.36	0.00	1	-3.40	-1.65	0.95											
29 1HDA-B	30	1	-3.40	-2.31	0.00	1	-3.40	-1.88	0.93											
30 1HLB	30	2	-2.71	-1.46	3.51	7	-1.46	-0.88	0.57											
31 1HLM	30	29	-0.03	2.50	4.01	8	-1.32	-0.63	0.36											
32 1HSY	30	1	-3.40	-2.03	0.00	1	-3.40	-1.87	0.84											
33 1ITH-A	30	1	-3.40	-2.42	0.00	1	-3.40	-2.60	0.62											
34 1LHT	30	1	-3.40	-2.91	0.00	1	-3.40	-1.81	0.85											
35 1MBA	30	1	-3.40	-3.30	0.00	1	-3.40	-2.32	0.58											
36 1MBS	30	29	-0.03	1.58	1.82	3	-2.30	-1.33	0.67											
37 1MYG-A	30	1	-3.40	-2.40	0.00	1	-3.40	-1.71	0.82											
38 1MYJ-A	30	1	-3.40	-2.35	0.00	1	-3.40	-1.80	0.82											
39 1MYT	30	1	-3.40	-3.39	0.00	1	-3.40	-1.88	0.87											
40 2DHB-A	30	15	-0.69	-0.10	0.76	4	-2.01	-1.14	0.88											
41 2DHB-B	30	19	-0.46	0.36	0.86	2	-2.71	-1.29	0.83											
42 2LHB	30	1	-3.40	-3.10	0.00	1	-3.40	-3.95	0.18											
43 2PGH-A	30	15	-0.69	-0.44	0.71	2	-2.71	-1.23	0.88											
44 2PGH-B	30	16	-0.63	-0.33	0.77	2	-2.71	-1.23	0.87											
45 4SDH-A	30	1	-3.40	-5.20	0.00	1	-3.40	-3.69	0.43											
lattice_ssfit																				
46 1BEO	2001	1	-7.60	-15.36	0.00	1	-7.60	-8.87	0.04	1	-10.1					1	-9.4			
47 1CTF	2001	1	-7.60	-12.44	0.00	1	-7.60	-7.19	-0.04	1	-6.6			1	-6.17	1	-6.7		1	-7.86
48 1DKT-A	2001	1	-7.60	-9.50	0.00	1	-7.60	-9.59	0.02	1	-5.4			2	-3.92	1	-5.6		1	-5.35
49 1FCA	2001	1	-7.60	-10.59	0.00	1	-7.60	-8.26	0.01	1	-5.1			36	-2.25	1	-5.6		1	-5.13
50 1NKL	2001	1	-7.60	-8.36	0.00	1	-7.60	-7.69	-0.02	1	-7.8			1	-4.51	1	-7.3		1	-6.22
51 1PGB	2001	1	-7.60	-14.19	0.00	1	-7.60	-8.39	-0.01	1	-9.9			1	-4.13	1	-8.9		1	-6.15
52 1TRL-A	2001	1	-7.60	-9.31	0.00	1	-7.60	-7.62	-0.01	1	-4.9			1	-3.63	1	-3.9		1	-6.58
53 4ICB	2001	1	-7.60	-9.20	0.00	1	-7.60	-6.03	-0.03	1	-4.9					1	-4.3			
lmds																				
54 1B0N-B	498	1	-6.21	-5.05	0.00	1	-6.21	-5.31	0.14											
55 1BBA	501	203	-0.90	-0.24	3.29	37	-2.61	-1.54	0.30	35	-1.5					501	9.4			
56 1CTF	498	1	-6.21	-7.31	0.00	1	-6.21	-4.50	0.21	1	-3.4			1	-4.13	1	-3.7		1	-5.70
57 1DTK	216	1	-5.38	-4.07	0.00	1	-5.38	-5.55	0.11	10	-1.8			5	-1.88	23	-1.3		24	-1.26
58 1FC2	501	501	0.00	3.25	5.90	351	-0.36	0.41	-0.07	3	-2.6			14	-2.04	499	2.7		56	-1.26
59 1IGD	501	1	-6.22	-8.62	0.00	1	-6.22	-4.64	0.32	1	-3.4			2	-3.11	1	-5.0		1	-3.20
60 1SHF-A	438	1	-6.08	-10.55	0.00	1	-6.08	-7.27	0.05	1	-5.6			1	-4.13	1	-4.5		1	-5.54
61 2CRO	501	1	-6.22	-7.20	0.00	1	-6.22	-5.09	0.04	12	-3.1			1	-3.96	359	0.6		1	-4.77
62 2OVO	348	1	-5.85	-6.65	0.00	1	-5.85	-6.67	0.10	3	-2.5			1	-3.62	18	-1.7		1	-3.94
63 4PTI	344	1	-5.84	-6.96	0.00	1	-5.84	-5.19	0.16	16	-1.6					12	-1.7			
lmds_v2																				
64 1BBA	101	65	-0.44	0.33	5.59	62	-0.49	0.11	0.06											
65 1CTF	101	1	-4.62	-6.59	0.00	1	-4.62	-3.90	0.26											
66 1FC2	101	97	-0.04	1.80	6.06	45	-0.81	-0.33	0.12											
67 1GPT	101	1	-4.62	-2.69	0.00	1	-4.62	-3.43	0.32	2	-2.0					4	-1.8			
68 1IGD	101	1	-4.62	-7.21	0.00	1	-4.62	-4.09	0.25											
69 1SHF-A	101	1	-4.62	-7.43	0.00	1	-4.62	-4.95	0.18											
70 1UBI	301	1	-5.71	-10.31	0.00	1	-5.71	-7.23	0.13	1	-4.3					1	-4.3			
71 2CRO	101	1	-4.62	-5.75	0.00	1	-4.62	-4.30	0.25											
72 2OVO	101	1	-4.62	-5.55	0.00	1	-4.62	-4.89	0.14											
73 4PTI	101	1	-4.62	-6.94	0.00	1	-4.62	-6.80	0.12											
semfold																				
74 1CTF	11401	1	-9.34	-5.61	0.00	1	-9.34	-6.88	0.03											
75 1E68	11361	1	-9.34	-3.30	0.00	1	-9.34	-4.54	0.10											
76 1EH2	11441	2	-8.65	-3.08	11.75	5327	-0.76	0.08	0.08											
77 1KHM	21081	1	-9.96	-4.97	0.00	1	-9.96	-5.96	0.06											
78 1NKL	11661	1332	-2.17	-1.21	3.98	6	-7.57	-3.66	0.18											
79 1PGB	11281	1	-9.33	-4.96	0.00	1	-9.33	-7.68	0.02											

[a] Taken from Reference[25]

[b] The potential developed by Reference[24].

[c] the potential developed by Reference[13] and taken from Reference[25].

[d] the potential developed by Reference[33].

TABLE VI: The performance of the present potential for each set of immunoglobulin decoys.

Decoy set		The present potential, $e^o + e^r + e^s$							
	#decoys	$rank_e$	$\log P_e$	Z_e	RMSD	$rank_r$	$\log P_r$	Z_r	R[a]
ig_structal									
1 1ACY	61	1	-4.11	-2.49	0.00	1	-4.11	-2.48	0.37
2 1BAF	61	1	-4.11	-3.07	0.00	1	-4.11	-2.33	0.35
3 1BBD	61	1	-4.11	-3.17	0.00	1	-4.11	-3.66	0.39
4 1BBJ	61	2	-3.42	-1.61	1.11	17	-1.28	-0.59	0.42
5 1DBB	61	9	-1.91	-0.97	1.11	3	-3.01	-1.23	0.44
6 1DFB	61	1	-4.11	-2.41	0.00	1	-4.11	-2.99	0.45
7 1DVF	61	1	-4.11	-4.19	0.00	1	-4.11	-2.02	0.32
8 1EAP	61	1	-4.11	-2.70	0.00	1	-4.11	-3.35	0.25
9 1FAI	61	16	-1.34	-0.60	3.19	52	-0.16	1.05	0.26
10 1FBI	61	9	-1.91	-1.06	1.84	24	-0.93	-0.45	0.52
11 1FGV	61	1	-4.11	-4.71	0.00	1	-4.11	-2.24	0.49
12 1FIG	61	61	0.00	4.58	1.66	12	-1.63	-0.69	0.40
13 1FLR	61	1	-4.11	-3.10	0.00	1	-4.11	-3.21	0.47
14 1FOR	61	1	-4.11	-3.66	0.00	1	-4.11	-2.06	0.38
15 1FPT	61	1	-4.11	-2.16	0.00	1	-4.11	-2.69	0.52
16 1FRG	61	1	-4.11	-3.57	0.00	1	-4.11	-2.69	0.50
17 1FVC	61	1	-4.11	-3.93	0.00	1	-4.11	-5.15	0.24
18 1FVD	61	1	-4.11	-3.77	0.00	1	-4.11	-2.25	0.36
19 1GAF	61	1	-4.11	-5.50	0.00	1	-4.11	-2.48	0.27
20 1GGI	61	1	-4.11	-1.91	0.00	1	-4.11	-2.37	0.25
21 1GIG	61	1	-4.11	-6.33	0.00	1	-4.11	-3.47	0.43
22 1HIL	61	1	-4.11	-4.63	0.00	1	-4.11	-2.63	0.59
23 1HKL	61	1	-4.11	-3.18	0.00	1	-4.11	-2.30	0.24
24 1IAI	61	1	-4.11	-2.34	0.00	1	-4.11	-2.40	0.52
25 1IBG	61	1	-4.11	-2.38	0.00	1	-4.11	-6.20	0.18
26 1IGC	61	14	-1.47	-0.67	1.29	13	-1.55	-0.63	0.48
27 1IGF	61	1	-4.11	-2.36	0.00	1	-4.11	-2.71	0.52
28 1IGI	61	1	-4.11	-2.73	0.00	1	-4.11	-6.10	0.50
29 1IGM	61	1	-4.11	-1.89	0.00	1	-4.11	-2.72	0.35
30 1IKF	61	1	-4.11	-4.62	0.00	1	-4.11	-2.80	0.47
31 1IND	61	1	-4.11	-6.35	0.00	1	-4.11	-3.57	0.18
32 1JEL	61	2	-3.42	-1.81	1.03	2	-3.42	-1.17	0.52
33 1JHL	61	1	-4.11	-3.25	0.00	1	-4.11	-4.74	0.25
34 1KEM	61	1	-4.11	-3.16	0.00	1	-4.11	-3.44	0.40
35 1MAM	61	1	-4.11	-2.58	0.00	1	-4.11	-5.50	0.20
36 1MCP	61	1	-4.11	-2.41	0.00	1	-4.11	-2.70	0.54
37 1MFA	61	1	-4.11	-7.37	0.00	1	-4.11	-6.04	0.22
38 1MLB	61	1	-4.11	-3.45	0.00	1	-4.11	-2.01	0.49
39 1MRD	61	1	-4.11	-3.65	0.00	1	-4.11	-5.55	0.45
40 1NBV	61	51	-0.18	0.69	1.21	2	-3.42	-1.35	0.34
41 1NCB	61	1	-4.11	-1.75	0.00	1	-4.11	-2.84	0.39
42 1NGQ	61	1	-4.11	-6.25	0.00	1	-4.11	-4.18	0.39
43 1NMB	61	1	-4.11	-2.12	0.00	1	-4.11	-5.27	0.22
44 1NSN	61	58	-0.05	1.96	3.10	55	-0.10	1.75	0.19
45 1OPG	61	1	-4.11	-2.17	0.00	1	-4.11	-2.97	0.38
46 1PLG	61	1	-4.11	-3.87	0.00	1	-4.11	-2.69	0.49
47 1RMF	61	25	-0.89	-0.36	1.67	5	-2.50	-0.84	0.41
48 1TET	61	1	-4.11	-3.94	0.00	1	-4.11	-2.47	0.47
49 1UCB	61	1	-4.11	-4.17	0.00	1	-4.11	-2.86	0.22
50 1VFA	61	1	-4.11	-5.57	0.00	1	-4.11	-4.87	0.17
51 1VGE	61	1	-4.11	-4.96	0.00	1	-4.11	-6.18	0.20
52 1YUH	61	41	-0.40	0.31	2.53	52	-0.16	0.42	0.07
53 2CGR	61	1	-4.11	-4.35	0.00	1	-4.11	-2.47	0.43
54 2FB4	61	1	-4.11	-5.07	0.00	1	-4.11	-3.24	0.36
55 2FBJ	61	1	-4.11	-3.81	0.00	1	-4.11	-2.53	0.08
56 2GFB	61	1	-4.11	-3.82	0.00	1	-4.11	-5.35	0.17
57 3HFL	61	1	-4.11	-2.31	0.00	1	-4.11	-5.61	0.40
58 3HFM	61	59	-0.03	1.68	1.09	5	-2.50	-0.80	0.36
59 6FAB	61	1	-4.11	-4.11	0.00	1	-4.11	-2.55	0.52
60 7FAB	61	1	-4.11	-5.31	0.00	1	-4.11	-4.27	0.32
61 8FAB	61	1	-4.11	-5.94	0.00	1	-4.11	-6.74	0.02
ig_structal_hires									
62 1DVF	20	1	-3.00	-3.41	0.00	1	-3.00	-1.92	0.54
63 1FGV	20	1	-3.00	-4.52	0.00	1	-3.00	-2.24	0.60
64 1FLR	20	1	-3.00	-2.99	0.00	1	-3.00	-2.85	0.71
65 1FVC	20	1	-3.00	-3.44	0.00	1	-3.00	-4.43	0.10
66 1GAF	20	1	-3.00	-5.32	0.00	1	-3.00	-2.43	0.28
67 1HIL	20	1	-3.00	-4.60	0.00	1	-3.00	-2.61	0.74
68 1IND	20	1	-3.00	-8.00	0.00	1	-3.00	-3.76	0.17
69 1KEM	20	1	-3.00	-2.89	0.00	1	-3.00	-3.09	0.37
70 1MFA	20	1	-3.00	-8.82	0.00	1	-3.00	-5.56	0.14
71 1MLB	20	1	-3.00	-3.20	0.00	1	-3.00	-2.13	0.81
72 1NBV	20	16	-0.22	0.46	1.72	7	-1.05	-0.55	0.45
73 1OPG	20	1	-3.00	-1.98	0.00	1	-3.00	-3.01	0.44
74 1VFA	20	1	-3.00	-4.56	0.00	1	-3.00	-4.75	0.35
75 1VGE	20	1	-3.00	-4.69	0.00	1	-3.00	-6.34	0.04
76 2CGR	20	1	-3.00	-5.61	0.00	1	-3.00	-2.67	0.56
77 2FB4	20	1	-3.00	-5.71	0.00	1	-3.00	-4.26	0.75
78 2FBJ	20	1	-3.00	-3.89	0.00	1	-3.00	-2.42	0.48
79 6FAB	20	1	-3.00	-3.48	0.00	1	-3.00	-2.56	0.69
80 7FAB	20	1	-3.00	-4.59	0.00	1	-3.00	-4.22	0.40
81 8FAB	20	1	-3.00	-5.01	0.00	1	-3.00	-4.80	-0.04

[a] R is the correlation coefficient of rank order between the energies and RMSDs of decoys in a decoy set.