

Table S5. Shift and tightening values for each distribution generated by HC/LC docking

Antibody	HL shift	HC1 shift	LC1 shift	HC2 shift	LC2 shift	dc shift	HL Tightening	HC1 Tightening	LC1 Tightening	HC2 Tightening	LC2 Tightening	dc Tightening
VRC01	3.30	1.27	3.79	0.46	4.13	0.11	0.78	1.08	0.73	0.33	0.59	1.08
VRC03	5.96	1.07	2.20	1.71	5.19	0.39	1.27	1.80	0.55	1.14	0.90	0.87
VRC-PG04	0.18	1.01	0.37	1.07	0.98	0.56	0.37	0.49	0.32	0.63	0.56	1.31
VRC23	4.40	0.81	1.43	1.48	3.44	0.21	2.98	1.24	1.89	1.33	0.63	1.78
VRC06	1.49	0.42	1.78	0.93	2.13	0.02	0.68	0.65	0.61	0.98	1.21	1.40
12a12	0.20	4.05	2.34	3.70	6.17	1.18	0.49	6.58	1.51	2.23	2.21	1.88
VRC-PG20	0.89	0.20	0.22	0.49	2.20	0.00	0.72	0.42	0.51	0.46	0.56	0.50
VRC07	2.57	0.10	2.25	0.51	1.82	0.03	0.69	0.93	0.83	1.09	1.10	0.87
8ANC131	1.37	0.80	2.51	1.37	1.80	0.37	15.46	17.01	17.62	11.06	1.76	2.22