

Supplementary Data

SUPPLEMENTARY TABLE S1. ALIGNED PRE/POSTFUSION INFLUENZA HA CHAIN F

<i>Residue</i>	ϕ_{pre}	ψ_{pre}	ϕ_{post}	ψ_{post}	$\Delta\phi$	$\Delta\psi$	Π_{pre}	Π_{post}
40	-69	-34.4	-69	-71.6	0	37.2	0.85	9.85
41	-60.2	-42.2	-39.4	-53.7	20.8	11.5	4.18	0.7
42	-68	-43.9	-59	-38	9	5.9	2.73	2.15
43	-53.7	-47.9	-74.6	-32.2	20.9	15.7	3.34	3.26
44	-63.2	-49.3	-60.9	-53.9	2.3	4.6	1.46	9.85
45	-62.4	-44	-61.8	-29.4	0.6	14.6	0.85	9.02
46	-59.3	-48	-73.6	-31.4	14.3	16.6	4.18	1.56
47	-57.1	-44.1	-71.3	-46.1	14.2	2	2.73	3.41
48	-66.5	-36.9	-54	-58.3	12.5	21.4	3.34	4.77
49	-68.5	-34	-63	-30.9	5.5	3.1	4.06	3.63
50	-62.3	-50.5	-76.5	-22.1	14.2	28.4	0.68	9.02
51	-67.3	-37.6	-82.7	-43.3	15.4	5.7	2.43	2.73
52	-59	-42.2	-59	-37.3	0	4.9	1.28	9.85
53	-69.7	-36.6	-78.8	-18.6	9.1	18	2.3	3.09
54	-64.5	-35.3	-71.1	-37.7	6.6	2.4	6.87	4.83
55	-70.6	-38.4	-69.3	-66	1.3	27.6	0.39	5.1
56	-86.1	10.8	-44.7	-44.3	41.4	55.1	1.56	8.35
57	-62.5	-163.4	-61.9	-49.6	0.6	113.8	0.39	9.85
58	-57.1	125.2	-66.6	-40	9.5	165.2	6.87	3.09
59	-74.1	135.8	-61	-60.1	13.1	164.1	0	8.7
60	-83.1	140.5	-40.7	-42	42.4	177.5	0	5.1
61	107.8	141.2	-72.9	-38.6	179.3	179.8	0	8.35
62	130.9	146.5	-64.2	-49.8	164.9	163.7	9.85	4.55
63	112.8	-109.2	-50.8	-34.1	163.6	75.1	0	8.7
64	-67.7	123.7	-74.1	-36.1	6.4	159.8	0	4.93
65	125.5	-140.4	-74.2	-25	160.3	115.4	0	2.35
66	102.4	162.3	-69.7	-47.9	172.1	149.8	0	2.12
67	-72	149.9	-58.5	-39.4	13.5	170.7	0	5.35
68	129.1	8.7	-63.2	-45.2	167.7	53.9	0	2.35
69	144	135.6	-65.9	-38.4	150.1	174	0	1.03
70	128.8	146.2	-58.1	-38	173.1	175.8	0	6.22
71	118.3	15.8	-72.3	-39	169.4	54.8	0	3.47
72	141.9	155.8	-58.6	-44.5	159.5	159.7	0	2.66
73	-98.8	122.3	-63.6	-60.4	35.2	177.3	0	5.48
74	119.9	-24.6	-57.7	-23.4	177.6	1.2	0	4.64
75	94.7	-135	-76.8	-45.1	171.5	89.9	6.48	6.22
76	-52.6	-53.3	-65.8	-27.4	13.2	25.9	0.44	3.47
77	-67.3	-36.6	-69.9	-34.3	2.6	2.3	0.6	1.88
78	-71	-35.3	-75.6	-36.7	4.6	1.4	1.55	5.48
79	-58.6	-40.8	-60.4	-37.7	1.8	3.1	0.39	4.64
80	-69.6	-37.3	-68.7	-43.6	0.9	6.3	6.48	3.47
81	-63.1	-43.1	-58	-44.5	5.1	1.4	2.37	1.55
82	-67.6	-39.4	-64.7	-44.4	2.9	5	2.4	2.8
83	-65.4	-45.4	-69.2	-24.3	3.8	21.1	1.55	3.34
84	-55	-43.4	-71.6	-50.5	16.6	7.1	0.68	2.43
85	-76.9	-35.4	-52.6	-52.6	24.3	17.2	2.45	6.03
86	-70	-36	-62.5	-45.5	7.5	9.5	3.68	3.39
87	-75.2	-26.3	-55.6	-39.5	19.6	13.2	2.4	8.35
88	-63.4	-46.8	-67	-63.9	3.6	17.1	1.15	5.53

(continued)

SUPPLEMENTARY TABLE S1. (CONTINUED)

<i>Residue</i>	ϕ_{pre}	ψ_{pre}	ϕ_{post}	ψ_{post}	$\Delta\phi$	$\Delta\psi$	Π_{pre}	Π_{post}
89	-62.5	-49.7	-50.1	-32.4	12.4	17.3	3.27	4.05
90	-61.6	-33.5	-64.9	-54.1	3.3	20.6	1.28	6.03
91	-68.3	-43	-61.3	-36.1	7	6.9	3.68	3.39
92	-70.3	-29.1	-71	-40.5	0.7	11.4	3.34	8.35
93	-71.9	-36.1	-66.8	-37.4	5.1	1.3	0.87	5.53
94	-61.9	-48.4	-57.1	-39.7	4.8	8.7	3.27	4.05
95	-56.4	-51.5	-56.1	-55	0.3	3.5	1.59	4.77
96	-61.9	-34.4	-60.8	-30.8	1.1	3.6	7.95	4.92
97	-71.8	-40.1	-79	-28.9	7.2	11.2	3.34	4.12
98	-72.4	-35.8	-75.1	-31.1	2.7	4.7	1.89	4.68
99	-59.9	-59.1	-58.8	-48.8	1.1	10.3	5.2	5.58
100	-62.7	-32.4	-64.6	-45.9	1.9	13.5	3.17	2.43
101	-61.2	-51.5	-68.2	-21.1	7	30.4	7.95	4.92
102	-62.3	-53.2	-81.2	-46.8	18.9	6.4	2.31	9.85
103	-47.4	-50.5	-52.6	-49.2	5.2	1.3	1.89	8.74
104	-66.6	-38.1	-59.3	-36.9	7.3	1.2	5.2	1.64
105	-63.7	-44.1	-80.2	3.8	16.5	47.9	3.17	2.21
106	-69.8	-37.5	67.6	10.3	137.4	47.8	1.47	3.29
107	-61.1	-42.5	-67.4	-11.3	6.3	31.2	2.04	8.74
108	-65.5	-36.3	-159.3	176.1	93.8	147.6	0.66	9.85
109	-77	-33.8	-144.2	111.8	67.2	145.6	2.01	4.23
110	-60.7	-48.8	-66.7	11.5	6	60.3	2.21	0
111	-68.6	-32.1	-94.2	-30.4	25.6	1.7	2.33	0
112	-61.4	-44.4	-54.9	118.5	6.5	162.9	3.76	6.86
113	-56.1	-54.3	-40.2	-45.6	15.9	8.7	3.6	4.23
114	-58	-39.5	-63.4	-45.8	5.4	6.3	2.01	6.89
115	-59.7	-52.4	-74.5	-37.4	14.8	15	3.29	2.8
116	-61.9	-34.7	-62.1	-29.6	0.2	5.1	2.33	6.86
117	-66.7	-42.2	-66.9	-49.9	0.2	7.7	3.76	7.08
118	-58.9	-43.9	-48.4	-51.9	10.5	8	3.6	3.95
119	-57.2	-51.1	-59.6	-45.5	2.4	5.6	2.01	6.89
120	-63.9	-36.2	-67.8	-10.9	3.9	25.3	3.29	2.8
121	-67.2	-44.2	-75.4	-57.8	8.2	13.6	0.94	3.18
122	-64.4	-41.4	-60	-41.1	4.4	0.3	0.68	6.25
123	-58.2	-47.2	-56.5	-30.8	1.7	16.4	1.56	7.79
124	-63.9	-34.2	-81.6	-21.7	17.7	12.5	4.46	3.87
125	-67.9	-40.9	-76.5	-45.5	8.6	4.6	0.85	6.96
126	-73.4	-9.1	-67.4	-57.7	6	48.6	9	3.98
127	40.7	-124	-47.6	-22.5	88.3	101.5	0.65	0.68
128	-88.8	14.3	-88.4	-60.6	0.4	74.9	4.46	7.79
129	-99.4	-3.7	-92	36.2	7.4	39.9	0	0
130	141.3	163.8	-172.7	160	46	3.8	9	6.96
131	130.4	147.8	-79.4	107.2	150.2	40.6	0	5.29
132	-75.1	131	-77.9	114.6	2.8	16.4	5.23	9.52
133	-94.5	4.7	-63.9	-40.7	30.6	45.4	0	0
134	74.8	7.6	124.6	-32.2	49.8	39.8	9.85	8.92
135	128.1	27.5	-100.1	21	131.8	6.5	7.83	0
136	86.2	-2.9	88.2	16.4	2	19.3	9.85	6.02
137	106.2	132.6	-111	145.6	142.8	13	0	8.92
138	-91.4	140.9	-131	136.5	39.6	4.4	0	4.02
139	-93.3	113.2	-96.8	109	3.5	4.2	5.23	9.52
140	-84.8	120.9	-95.1	112.2	10.3	8.7	5.68	5.66
141	-90.5	51.5	-88.5	142.6	2	91.1	0	4.93
142	170.6	164.3	-115.8	101.7	73.6	62.6	5.68	0

(continued)

SUPPLEMENTARY TABLE S1. (CONTINUED)

<i>Residue</i>	ϕ_{pre}	ψ_{pre}	ϕ_{post}	ψ_{post}	$\Delta\phi$	$\Delta\psi$	Π_{pre}	Π_{post}
143	-69.9	119.8	-64.7	-25.4	5.2	145.2	0	0
144	127.8	91.4	-113.2	106.5	119	15.1	0	0
145	-67.1	176.8	-74.1	178.9	7	2.1	7.29	2.74
146	-61.7	-24.1	-63.1	-29.5	1.4	5.4	2.51	4.73
147	-79	-32.7	-68.8	-58.8	10.2	26.1	3.02	3.16
148	-64	-46.9	-50	-51.1	14	4.2	2.73	4.41
149	-58.8	-42.1	-56	-29.4	2.8	12.7	4.65	0
150	-65.6	-32.3	-69	-44.5	3.4	12.2	2.64	7.01
151	-70.6	-28.5	-53.2	-41.7	17.4	13.2	6.14	6.4
152	-66.8	-44.7	-58.7	-12.2	8.1	32.5	3.02	4.41
153	-68.8	-35.9	-109.8	-49	41	13.1	2.73	4.06
154	-97.9	18.2	-45.4	-49.9	52.5	68.1	3.08	7.01
155	71.8	21	64.5	33.3	7.3	12.3	1.49	3.99
156	114.6	18.6	-95.8	136.6	149.6	118	4.62	6.4
157	-69.1	124.1	-153.6	106.6	84.5	17.5	6.14	9.85
158	-97.1	108.7	-66.3	85.1	30.8	23.6	4.65	0
159	-66.9	-28.8	-74.1	107.4	7.2	136.2	4.7	0
160	-64.3	-34.9	-72.4	147.9	8.1	177.2	6.99	9.85
161	-51.1	-34.8	-135.8	109.8	84.7	144.6	0	0
162	116.5	-0.9	-70.8	-0.9	172.7	0	0	0

DSSP files for 2HMG and 1HTM are aligned along their common residues, conformational angles $\phi_{\text{pre}}, \psi_{\text{pre}}$ pre-fusion and $\phi_{\text{post}}, \psi_{\text{post}}$ post-fusion are given, and differences $\Delta\phi$ and $\Delta\psi$ are computed. The maximum of the Π -values of the two prospective BHBs are reported Π_{pre} pre- and Π_{post} post-fusion.