

Table S5. Disulfide bond of the vaccine

Residue 1			Residue 2			Bond		
Chain	Seq #	AA	Chain	Seq #	AA	χ^3	kcal/mol	ΣB factor
A	7	CYS	A	32	LEU	+83.94	6.12	0.00
A	11	CYS	A	22	ALA	-115.82	3.92	0.00
A	13	THR	A	18	GLY	-59.28	6.49	0.00
A	13	THR	A	22	ALA	+124.22	5.73	0.00
A	15	GLY	A	18	GLY	-68.40	5.52	0.00
A	29	VAL	A	65	GLY	+87.26	2.18	0.00
A	37	TYR	A	54	PRO	+86.21	2.54	0.00
A	39	PRO	A	48	ALA	+118.66	7.40	0.00
A	41	LEU	A	72	ALA	-101.73	2.15	0.00
A	42	ILE	A	102	THR	-105.96	5.74	0.00
A	42	ILE	A	103	ASN	+125.95	7.55	0.00
A	45	ALA	A	145	TYR	-92.15	4.04	0.00
A	74	ALA	A	79	ASN	+110.12	3.21	0.00
A	75	ALA	A	78	HIS	-96.46	2.82	0.00
A	101	SER	A	104	ILE	+106.95	1.45	0.00
A	105	ARG	A	108	ALA	-76.66	4.11	0.00
A	146	GLY	A	319	SER	-60.29	3.86	0.00
A	148	ALA	A	319	SER	-94.87	3.59	0.00
A	157	TYR	A	169	TYR	+77.21	6.46	0.00
A	161	ALA	A	166	ARG	+73.94	4.76	0.00
A	162	GLY	A	293	GLY	-57.44	2.18	0.00
A	171	MET	A	296	MET	-72.83	4.56	0.00
A	183	ALA	A	186	ALA	+92.47	3.24	0.00
A	187	ALA	A	192	ALA	+107.89	2.26	0.00
A	188	VAL	A	191	ALA	+82.87	4.98	0.00
A	190	ARG	A	256	THR	+115.87	4.78	0.00
A	206	PRO	A	212	GLY	+117.43	5.90	0.00
A	216	GLY	A	220	ALA	-113.43	2.66	0.00
A	239	ALA	A	245	GLY	-84.72	2.18	0.00
A	261	ALA	A	266	PRO	+121.85	3.41	0.00
A	262	PHE	A	265	GLY	+96.58	2.73	0.00
A	280	ALA	A	298	ALA	+118.23	4.30	0.00
A	286	PRO	A	289	SER	-85.59	5.26	0.00
A	299	SER	A	303	GLY	-107.88	4.97	0.00
A	359	ALA	A	362	ARG	-72.08	3.27	0.00
A	390	PRO	A	394	LEU	-88.29	3.30	0.00
A	403	GLY	A	412	GLY	-58.91	4.63	0.00
A	433	VAL	A	445	GLY	+108.26	3.06	0.00
A	434	GLY	A	443	GLY	-112.56	5.70	0.00
A	449	THR	A	453	VAL	+121.69	6.53	0.00
A	450	GLY	A	453	VAL	+95.69	3.07	0.00
A	452	ALA	A	471	THR	+126.03	6.49	0.00
A	454	VAL	A	469	ILE	-77.84	5.68	0.00
A	465	GLY	A	490	ASN	-92.10	5.80	0.00
A	487	GLY	A	574	GLY	+101.85	2.25	0.00
A	503	GLY	A	567	GLY	-104.99	3.62	0.00
A	504	PRO	A	564	PRO	-86.59	3.65	0.00
A	510	PHE	A	598	GLY	+70.38	4.72	0.00
A	514	SER	A	552	ALA	+102.22	3.09	0.00
A	517	LYS	A	519	GLN	+124.88	6.52	0.00
A	524	PRO	A	530	THR	-115.53	6.74	0.00
A	527	GLY	A	809	LYS	-63.42	5.27	0.00

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Table S5. Continued

Residue 1			Residue 2			Bond		
Chain	Seq #	AA	Chain	Seq #	AA	χ^3	kcal/mol	ΣB factor
A	528	ILE	A	809	LYS	+113.56	0.94	0.00
A	536	LEU	A	541	GLY	+125.80	5.87	0.00
A	553	ALA	A	597	ALA	+121.51	3.59	0.00
A	554	ILE	A	779	GLN	+123.20	5.82	0.00
A	560	GLY	A	599	SER	+105.73	3.94	0.00
A	561	SER	A	565	GLY	-63.55	4.42	0.00
A	569	GLY	A	647	GLY	-69.89	2.81	0.00
A	571	ALA	A	639	LYS	+102.52	5.73	0.00
A	579	GLY	A	632	ARG	-89.31	7.78	0.00
A	604	PRO	A	613	THR	+106.02	3.37	0.00
A	605	GLY	A	650	PHE	-99.28	3.36	0.00
A	607	GLY	A	610	ALA	+118.60	6.29	0.00
A	611	ALA	A	640	GLN	+113.45	4.43	0.00
A	638	ASN	A	641	LYS	-87.14	3.28	0.00
A	656	LYS	A	748	GLY	-68.22	4.69	0.00
A	659	GLN	A	745	GLY	+94.99	1.43	0.00
A	674	GLY	A	730	HIS	-96.38	1.70	0.00
A	677	GLY	A	728	GLY	-101.10	4.67	0.00
A	678	THR	A	681	GLN	+124.60	8.09	0.00
A	697	LYS	A	711	GLY	+93.88	0.51	0.00
A	713	ASP	A	730	HIS	+84.66	6.55	0.00
A	715	LYS	A	728	GLY	+114.31	3.73	0.00
A	717	GLN	A	727	GLY	-94.08	3.92	0.00
A	752	GLY	A	852	TRP	-72.84	2.01	0.00
A	763	ASP	A	815	LYS	+96.72	1.97	0.00
A	766	GLY	A	844	ALA	-80.67	2.15	0.00
A	782	GLY	A	788	LEU	+120.81	6.71	0.00
A	802	ALA	A	805	ALA	-86.57	5.80	0.00
A	807	THR	A	832	GLN	-79.18	2.58	0.00
A	812	GLY	A	846	LYS	+101.43	5.17	0.00
A	829	LEU	A	877	LYS	+88.17	3.02	0.00
A	856	LEU	A	877	LYS	+108.03	4.70	0.00
A	863	LYS	A	873	GLY	+107.95	4.31	0.00
A	883	TYR	A	1002	ALA	+98.48	3.64	0.00
A	885	GLY	A	1001	ALA	+99.68	3.52	0.00
A	885	GLY	A	1002	ALA	-96.00	7.44	0.00
A	908	ALA	A	986	GLN	+99.03	3.90	0.00
A	927	SER	A	930	SER	-91.67	2.21	0.00
A	940	SER	A	967	ILE	-78.36	6.04	0.00
A	945	LEU	A	965	ALA	+117.54	3.92	0.00
A	947	MET	A	955	ALA	+95.60	7.56	0.00
A	949	GLY	A	959	VAL	-66.27	5.95	0.00
A	999	ARG	A	1004	THR	+106.88	2.84	0.00
A	1000	GLY	A	1007	LYS	+75.82	3.29	0.00
A	1001	ALA	A	1007	LYS	-80.34	5.34	0.00
A	1002	ALA	A	1006	ALA	+100.50	1.73	0.00
A	1003	GLY	A	1006	ALA	-64.17	4.32	0.00
A	1028	MET	A	1057	SER	+99.64	0.70	0.00
A	1033	ALA	A	1056	LEU	+104.32	4.28	0.00
A	1045	TYR	A	1048	ALA	+125.46	6.12	0.00