

A multi-epitope-based vaccine designed by targeting cytoadherence proteins of *Mycoplasma gallisepticum*

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Supplementary Table 1: List of predicted MHC I binding epitopes

S.No	Protein	Allele	Peptide	1-log50k(aff)*	Affinity(nM)#	%Rank		
1.	GapA	HLA-B40:06	QEFTGFDAL	0.417	549.34	0.50		
			FEKEITAAV	0.488	253.54	0.20		
			KEITAAVNV	0.493	242.26	0.17		
			FENKINDIV	0.439	431.64	0.40		
			GEYVAVPQA	0.581	93.27	0.05		
		HLA-B41:04	QEFTGFDAL	0.582	92.19	0.17		
			LETQTTPL	0.530	162.13	0.40		
			VESLFTTAL	0.566	109.23	0.25		
			KEITAAVNV	0.516	187.13	0.50		
			GEYVAVPQA	0.518	184.30	0.40		
		HLA-B41:03	QEFTGFDAL	0.666	37.11	0.12		
			LETQTTPL	0.672	34.77	0.10		
			VESLFTTAL	0.682	31.21	0.07		
			FEKEITAAV	0.621	60.71	0.30		
		2.	PlpA	HLA-B40:06	YEYPEYEEI	0.427	492.48	0.40
					LENQYPPA	0.516	188.31	0.50
HLA-B41:03	YEYPEYEEI			0.601	74.57	0.50		
	IESQLQALL			0.649	44.84	0.17		
	FEKLMLANM			0.610	68.01	0.40		
HLA-B41:04	IESQLQALL			0.503	216.28	0.50		
	FEKLMLANM			0.513	193.54	0.50		

			LENQYYPPA	0.516	187.77	0.50		
3.	Hlp3	HLA-B40:06	AEVQPEPVV	0.435	451.94	0.40		
			QEYDYPPA	0.583	91.54	0.50		
			RQLGMIEPV	0.413	572.43	0.50		
			AEFRSRTLA	0.490	250.27	0.20		
		HLA-B41:03	QELLYNVI	0.602	74.16	0.50		
			AEQVEQQPV	0.625	57.82	0.30		
			QETKHHHAL	0.663	38.54	0.12		
		HLA-B41:04	QELLYNVI	0.588	86.16	0.17		
			AEQVEQQPV	0.545	137.63	0.30		
			QETKHHHAL	0.560	117.14	0.25		
			QEYDYPPA	0.538	147.88	0.40		
			AEFRSRTLA	0.514	192.48	0.50		
		4.	CrmA	HLA-B40:06	NEIGVILPL	0.518	184.51	0.12
					HLA-B41:03	NEIGVILPL	0.693	27.86
	GEIVNDFIL			0.621	60.60	0.30		
HLA-B41:04	NEIGVILPL			0.594	80.45	0.15		
	RQTRAYYAL			0.591	83.36	0.17		

Supplementary Table 2: List of MHCII binding epitopes

S.No	Protein	Allele	Peptide	Core peptide	1-log _{50k} (affinity)*	Binding Affinity(nM)#	%Rank
1.	GapA	DRB1_1	IRLRLVIDRSRAT	LLVIDRSRA	0.660	39.48	0.09

		482	N				
		DRB1_1 445	IRLRLVIDRSRAT N	LLVIDRSRA	0.560	117.07	0.12
			NPRNILNALTTAK GF	LNALTTAKG	0.464	328.57	2.00
			PFEKEITAAVNVR SL	ITAAVNRS	0.462	336.19	2.00
		DRB1_1 366	IRLRLVIDRSRAT N	LLVIDRSRA	0.780	10.84	0.40
		DRB1_1 310	IRLRLVIDRSRAT N	LLVIDRSRA	0.731	18.29	0.70
2.	PlpA	DRB1_1 445	KTFSLNKGLNKVII R	LNKGLNKVI	0.467	320.42	1.80
		DRB1_1 310	KTFSLNKGLNKVII R	LNKGLNKVI	0.700	25.58	1.60
3.	Hlp3	DRB1_1 482	KIHNKILKNLAKL KK	ILKNLAKLK	0.601	75.28	0.60
			NQTFNLIKPVFKFL K	FNLIKPVFK	0.556	121.44	1.80
			RPTYGLRRVSRIPS L	LRRVSRIPS	0.556	121.99	1.80
		DRB1_1 445	KIHNKILKNLAKL KK	ILKNLAKLK	0.523	173.55	0.40
			RPTYGLRRVSRIPS L	LRRVSRIPS	0.470	309.43	1.70
		DRB1_1 366	KIHNKILKNLAKL KK	ILKNLAKLK	0.782	10.61	0.40
			QTFNLIKPVFKFLK K	FNLIKPVFK	0.731	18.28	1.90

			YGLRRVSRIPSLAP R	LRRVSRIPS	0.732	18.15	1.90
		DRB1_1 310	KIHNKILKNLAKL KK	ILKNLAKLK	0.728	19.06	0.80
4.	CrmA	DRB1_1 445	FSRLYLNSVNSLSF I	LYLNSVNSL	0.477	286.75	1.40
			ATTYLRSQIGLAR TS	LRSQIGLAR	0.468	317.79	1.80
			PGDQFSSIKNIRTIF	FSSIKNIRT	0.471	305.49	1.70
			SVYKKIITQTANV KK	IITQTANVK	0.464	328.38	2.00
		DRB1_1 366	FSRLYLNSVNSLSF I	LYLNSVNSL	0.743	16.09	1.40
			PGDQFSSIKNIRTIF	FSSIKNIRT	0.744	16.00	1.40
		DRB1_1 310	FSRLYLNSVNSLSF I	LYLNSVNSL	0.730	18.57	0.70
			EIVNDFILDAPILP K	FILDAPILP	0.631	54.22	1.80
			LGFDGIRNNLNVG VK	IRNNLNVGV	0.654	42.06	1.10

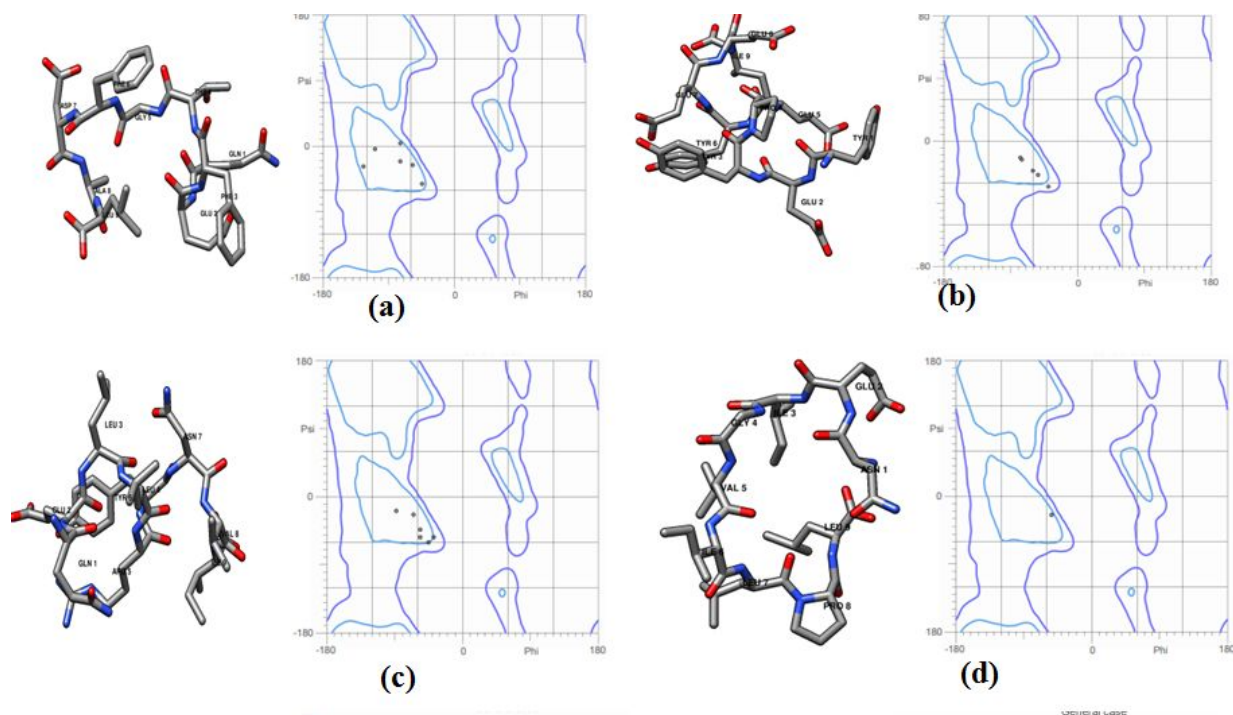
Supplementary Table 3: Models from Galaxy refine server

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotomers	Rama favored
MODEL 1	0.7832	0.820	4.049	126.8	5.7	60.8
MODEL 2	0.7883	0.821	4.052	117.5	6.3	60.8
MODEL 3	0.7793	0.838	4.100	122.3	7.0	60.8
MODEL 4	0.7908	0.828	4.127	117.2	8.2	62.4
MODEL 5	0.7806	0.822	3.998	124.3	5.1	61.3

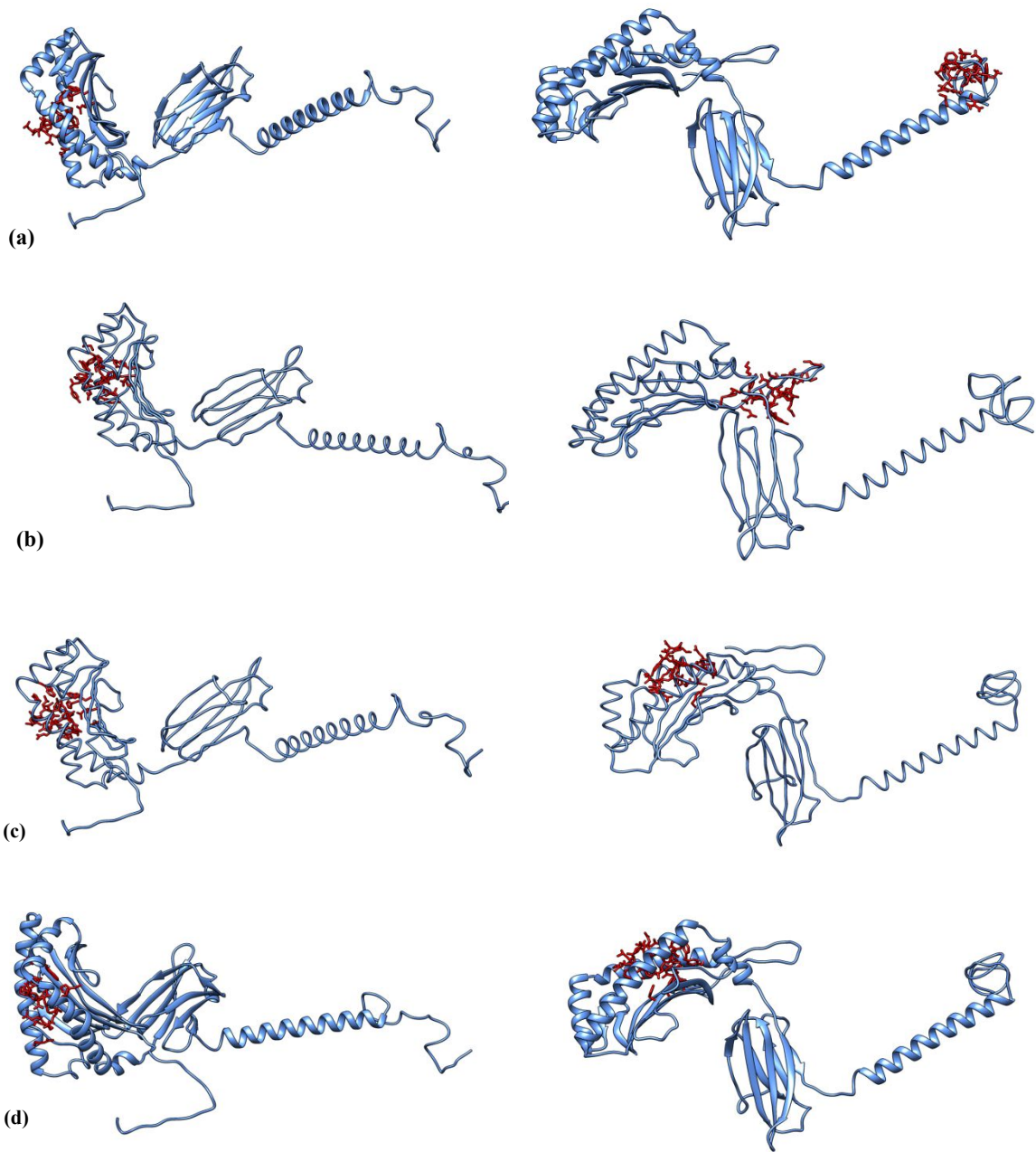
Supplementary Table 4: The binding energy and attractive VDW scores for suggested epitopes with chicken BF2 alleles using PatchDock

S.No	Protein	Ligand	Receptor	Global Energy kcal/mol	Attractive VDW kcal/mol
1.	GapA	QEFTGFDAL	BF2 2101	-44.69	-20.36
			BF2 0401	-6.25	-4.75
2.	PlpA	YEYPEYEEI	BF2 2101	-58.07	-27.10
			BF2 0401	-46.58	-22.33
3.	Hlp3	QELLRYNVI	BF2 2101	-44.73	-26.81
			BF2 0401	-44.05	-29.36

4.	CrmA	NEIGVILPL	BF2	-69.39	-27.93
			2101		
			BF2	-48.16	-29.74
			0401		



Supplementary Figure 1: Model and structure validation of epitopes (a) GapA (QEFTGFDAL), (b) PlpA (YEYPEYEEI), (c) Hlp3 (QELLRYNVI), (d) CrmA (NEIGVILPL).



Supplementary Figure 2: Docked complex of predicted epitopes with BF2 2101 and BF2 0401 alleles respectively. (a) GapA, (b) PlpA, (c) Hlp3, (d) CrmA