

Table S6. Simulation Parameters

Infection schedule, antigen and limiting factor presence			
symbol	default value	meaning	source / reason
t_{vacc}	[0, 28, 56]	Vaccination schedule in days	CHMI trial underlying this work [Mordmüller 2017]
τ_{decay}	2 days	Time constant of exponential Ag decay/removal in the system	[Mandel 1980]
p_{base}	0.005	Base activation probability per free B cell and timestep	choice leading to 10% activation
$t_{\text{GC,max}}$	day 7	Day until which the GC stays at maximum size	onset of <i>Pf</i> blood stage [Keitany 2016]
$\tau_{\text{GC decay}}$	10 days, <i>varies</i>	Time constant of exponential limiting factor decay after $t_{\text{GC,max}}$	set to reduce GC size faster than normal [Wittenbrink 2011, Weisel2016] due to blood stage antigens [Keitany 2016]
GC dynamics			
symbol	default value	meaning	source / reason
t_{init}	3 days	Time needed by B cells to become fully activated and migrate to the follicle to form a GC after initial antigenic contact	[DeSilva 2015]
t_{AID}	3 days	Time needed for cells having newly joined the GC before they start acquiring mutations during divisions	[Kleinstein 2003]
t_{help}	2 hours	Time that selected B cells receive survival signals before deciding to divide or differentiate	order of [Allen 2007 Science 315] (several contacts of 10-60 min)
n_{div}	2	number of divisions B cells undergo following selection	mean in [Gitlin 2014]
t_{div}	8 hours	Time needed for cell division in the GC after having received survival signal	[Allen 2007 Immunity 27]
t_{diff}	8 hours	Time needed for differentiation into a memory cell after having received survival signal	chosen to match t_{div}
$t_{\text{life, GC}}$	8 hours	Maximum survival time of GC cells in the waiting area	choice with minor effect on results
$t_{\text{life, naive}}$	14 days	Lifetime of naïve cells that have not been activated; new naïve cells are continuously introduced into the simulation to keep up the poolsize n_{naive}	[Macallan 2012]
r	0.9	Fraction of cells choosing to divide and recycle instead of leaving as a differentiated cell after receiving survival signal	[Meyer 2012]
p_{PC}	0.5	Fraction of exported cells that are of plasma cell phenotype, $1-p_{\text{PC}}$ are exported as memory; plasma cells are not modeled explicitly, thus cells in question are removed from the system	[Chaudhury 2014]

Binding model & mutations

symbol	default value	meaning	source / reason
n_{key}	[1 ... 15]	Number of residues jointly determining affinity towards a given epitope sequence	text
n_V	220	Combined length of the V_H and V_L segments	
b^{thr}	0.6	Binding threshold in normalized energy units	text
K_D^{thr}	10^{-5} M	Corresponding binding threshold as dissociation constant	[Batista1998], [Childs 2015]
b^{top}	1	Maximum binding strength in normalized energy units	text
K_D^{top}	10^{-9} M	Corresponding maximum binding strength as dissociation constant	[Batista1998], [Childs 2015]
p_{err}	0.003	Error probability per codon and division	[McKean 1984, Kleinstein 2003]
p_{death}	0.5	Probability that a replacement mutation in a residue relevant for stability leads to a non-functional Ab (and hence cell death)	[Kleinstein 2003]
p_{block}	0.55	Probability that a mutation in a non-key residue results in blocking of affinity maturation	mean of values given in [Kleinstein2003]

Simulation size

symbol	default value	meaning	source / reason
n_{GC}	50, <i>varies</i>	Number of individual GCs in the system	text, weak affect on results
n_{LF}	25, <i>varies</i>	Number of limiting factors (T_{FH} cells) per GC	leads to GCs of 500 cells in steady state, in range of [Wittenbrink2010]
n_{naive}	1000, <i>varies</i>	Steady state number of potentially binding free naïve cells per GC	
n_{freemem}	100	Number of binding free memory cells from former infections per GC at $t=0$	text
t_{step}	2 hours	Simulation timestep	chosen to match smallest simulated time unit (t_{help})