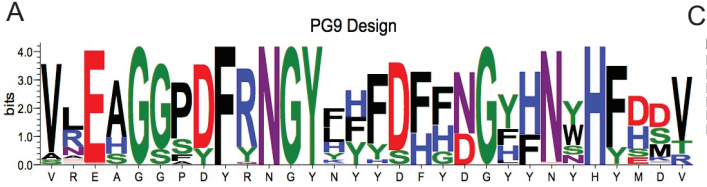

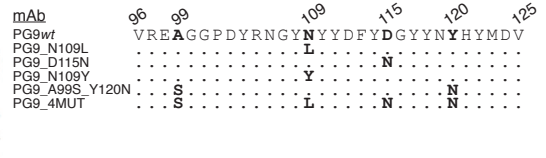

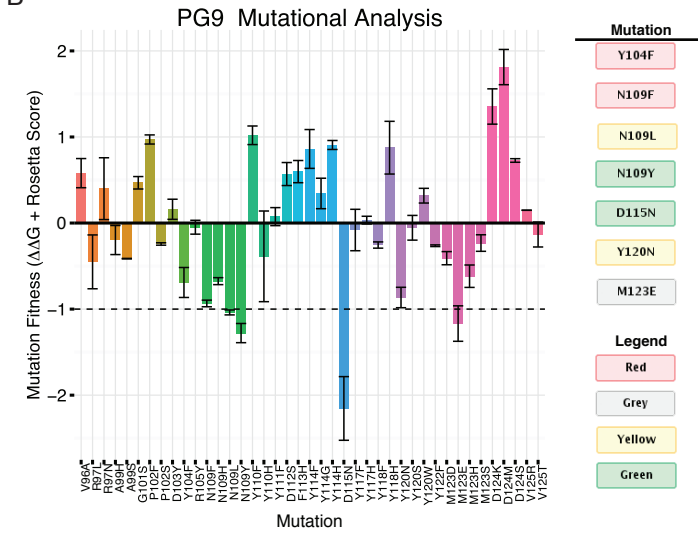

Mutation	Rosetta Justification
Y104F	*wt* tyrosine makes hydrogen bond with *wt* G107 backbone. The mutant 107F takes on the exact same side-chain configuration as the *wt tyrosine* but doesn't make the hydrogen contact to stablize the loop.
N109F	Mutant F109 makes a inter-HCDR3 hydrophobic stack contacted with a designed phenyalanine at position 104. It loses a hydrogen bond contact from a *wt* asparagine side-chain.
N109L	The leucine packs well if there is a mutated 111F, but the 111F is not preferred by Rosetta. However, it also packs against *wt* proline at position 102. Also packs against a lysine at position 40 on the antigen face.
N109Y	This mutatation packs against everything the 109L does and it has a polar group facing the solvent as well. The Dunbrack score is also highly favored.
D115N	Favored Rosetta Dunbrack. The hydrogen bonds are all retained by the mutant asparagine. Additional hydrogen bond made by the sp2 oxygen over to a glutamate at position 36 on the antigen. Rosetta prefers the polar NH2 group of the asparagine facing the solvent.
Y120N	The additional inter-HCDR3 loop hydrogen bonds that the mutant asparagine requires that positon 99 also be a mutant serine making this mutation cooperative. The *wt* tyrosine makes another inter-loop hydrogen bond with the backbone atoms to a *wt* proline 102.
M123E	The solvation is really poor but it makes an extra hydrogen bond with a wild-type tryptophan at position 126. It also makes another hydrogen bond with a mutant serine at position 96.

Legend

Red	Mutation predicted was not be beneficial, and was not tested
Grey	Mutation predicted to have no effect
Yellow	Mutation predicted to be beneficial, but needs to be paired with other mutations
Green	A single point mutation that was predicted to be beneficial