

Figure S1. RMSD values for all MD simulation runs.

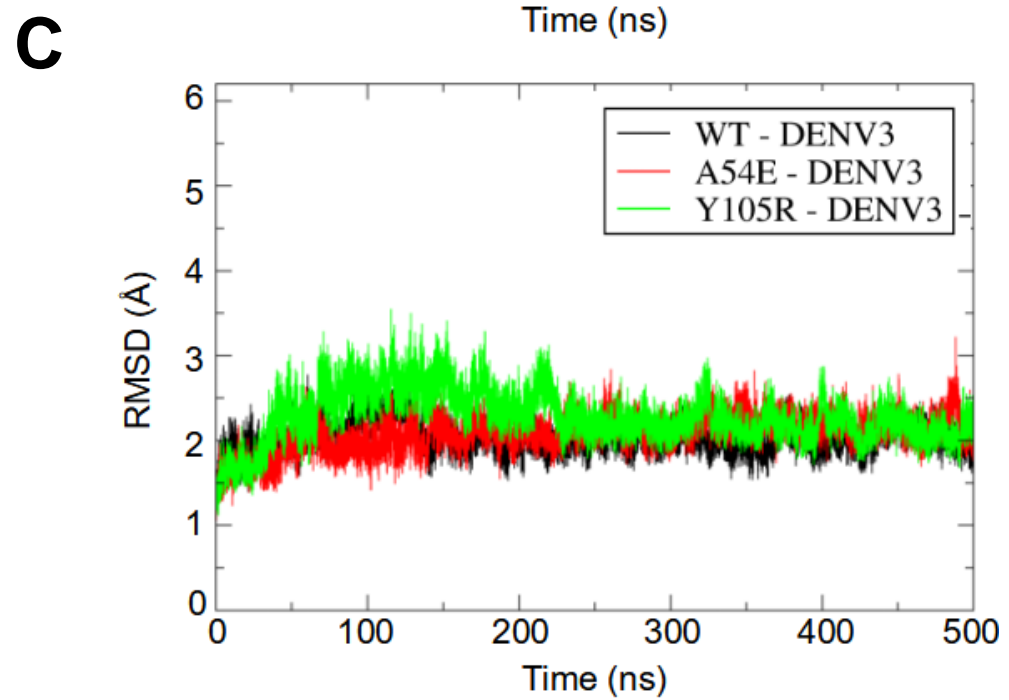
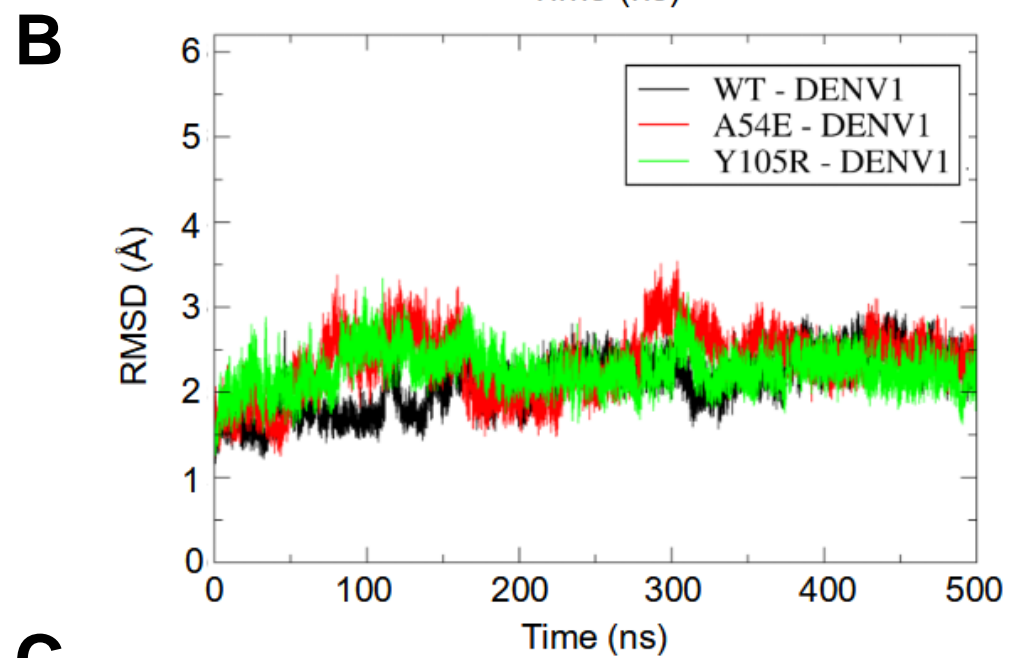
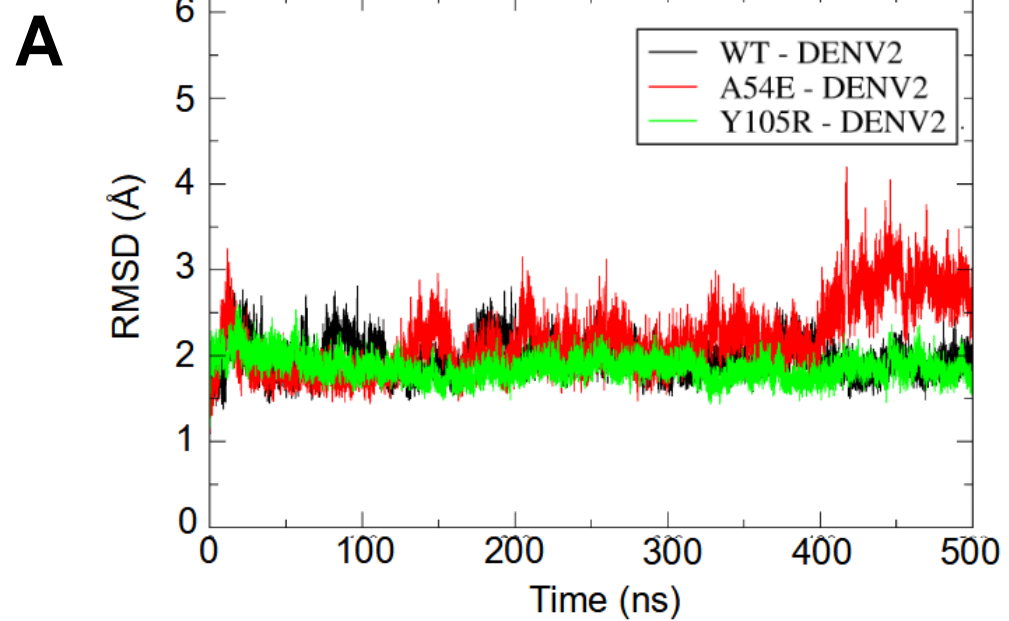


Figure S2. Energy contribution of residues that interacted with Lys325 in the Y105R.H – DENV3 EDIII complex. The plot corresponds to the heatmap in Figure 8A . The bars represent averages and solid lines represent the standard deviation. The EDIII, 1A1D-2 heavy chain and light chain are designated as A, H and L chain, respectively.

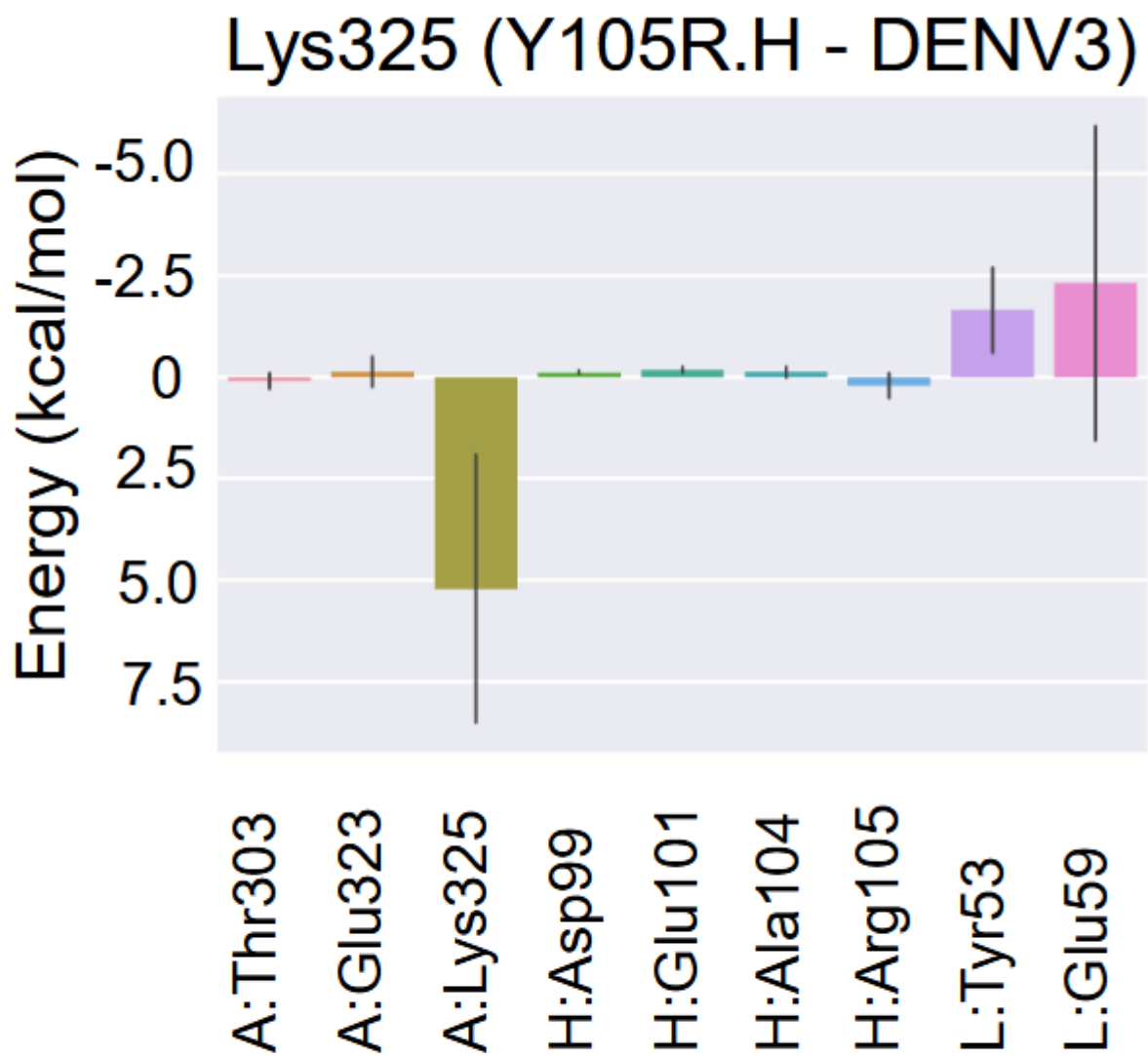


Figure S3. MD simulation of Y105R.H with DENV1 (0 to 500-ns). (A) Energy decomposition analysis: heat maps show energy contribution of residues that interact with Arg105.H per frame in the Y105R.H – DENV1 EDIII complex. Twenty frames with a 25-ns interval were extracted from the full simulation. Red arrows highlight residues strongly interacting with Arg105.H. (B) Energy contribution of residues that interacted with Arg105.H, corresponding to the heatmap in (A). The bars represent averages and solid lines represent the standard deviation. The EDIII, 1A1D-2 heavy chain and light chain are designated as A, H and L chain, respectively.

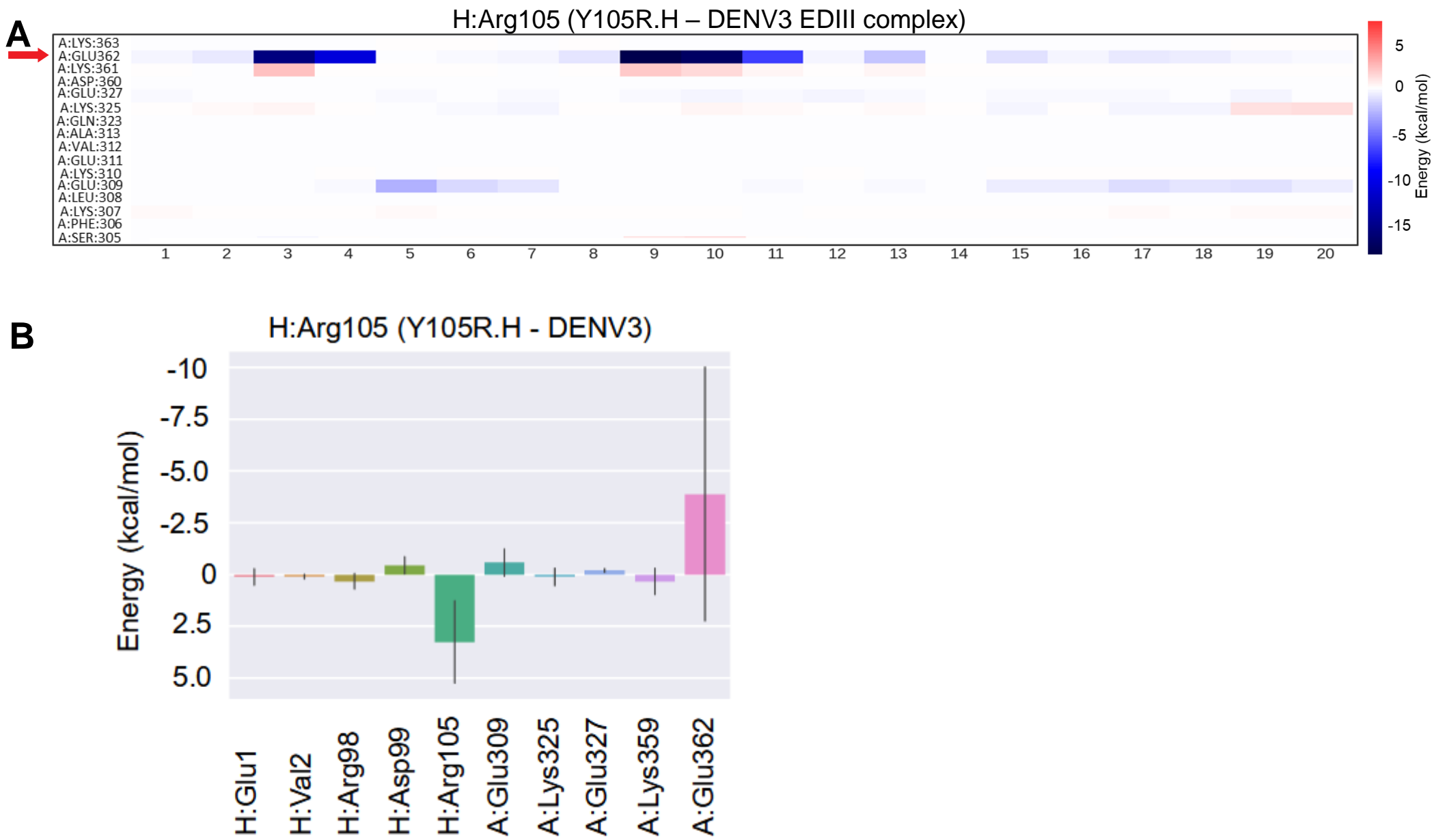


Table S1. List of primer pairs used for cloning and mutagenesis.

Primer Names	Sequence (5'→3')
Cloning	
pMal-c2X-DV1-F	GCAGACTAATTCGAGCTCCATGGGTATGAGCTAC
pMal-c2X-DV1-R	TGCCTGCAGGTCGACTCTAGATTATTAGCCTTTTTTTGAACCA
pMal-c2X-DV2-F	GCAGACTAATTCGAGCTCCAAAGGCATGTCTTAC
pMal-c2X-DV2-R	TGCCTGCAGGTCGACTCTAGATTATTAACCTTTTTTTGAACCA
pMal-c2X-DV3-F	GCAGACTAATTCGAGCTCCAAGGGCATGAGCTAC
pMal-c2X-DV3-R	TGCCTGCAGGTCGACTCTAGATTATTAGCCTTTACGGTACC
pMal-c2X-DV4-F	GCAGACTAATTCGAGCTCCAAAGGTATGAGCTAC
pMal-c2X-DV4-R	TGCCTGCAGGTCGACTCTAGATTATTAACCTTTACGGAACCA
Mutagenesis	
HCDR2-A54E-F	GATCCGGAAAACGGTTATTCTAAATATGACCCGAA
HCDR2-A54E-R	ACCGTTTTCCGGATCGATACGACCAATCCATTCCA
HCDR3-Y105R-F	GGTTTCGCGCGTTGGGGTCAGGGTACCCTGGTTAC
HCDR3-Y105R-R	CTGACCCCAACGCGCGGAAACCTTCGTAATCACGCG
Sequencing	
pComb3XSS-light-chain-F	AAGACAGCTATCGCGATTGCAG
pComb3XSS-light-chain-R	CGGCTGCCGTAGGCAATAGGT
pComb3XSS-heavy-chain-F	ACCTATTGCCTACGGCAGCCG
pComb3XSS-heavy-chain-R	AGAAGCGTAGTCCGGAACGTC