Structure and function of three human antibodies targeting the vaccinia virus adhesion molecule D8

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Table S1
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TABLE S1. D8 epitope residues and buried surface area.

Antibody	Chain	H-bond, salt bridge^{s}	VdW	BSA (Å^{2})
VACV-66	HC	Q3, Q4, H110, D111^{s}, D112, D179, D228^{s}, T229	N18, R20, L21, F56, P58, Y61, K109, H110, D112, I115, T168, L170, V181, E230, Y232	1776
	LC	R20	N18, A19	306
VACV-138	HC	T34, T35, Q37, R44^{s}, N46, K48, S65, Y104, E105, K108^{s}, N145, S147, N175	T39, S64, T146, P149	1432
	LC	N145	R142, S143, A144, L203	564
VACV-304	HC	T34, T35, N46, E105, S140, N145, S147	Q37, N38, T39, N46, F47, T146, A148, P149	1010
	LC	K48^{s}, K98, S102, Y104	T34, F47, W96, S103, P149, D151	977

TABLE S2. Antibody-antigen polar contacts

Antibody and H or L chain	D8 Antigen	CDR	Interaction[a]
VACV-66			
Ser30H^{O}	Gln3^{NE2}	H1	H
Asn32H^{OD1}	Gln4^{N}	H1	H
Asn32H^{ND2}	Gln4^{O}	H1	H
Asn32H^{ND2}	Gln3^{OE1}	H1	H
Asn32H^{ND2}	Asp179^{OD1}	H1	H
Asn33H^{ND2}	Thr229^{OG1}	H1	H
Tyr34H^{OH}	Asp228^{OD2}	H1	H
Tyr35H^{OH}	Asp111^{OD2}	H1	H
Tyr55H^{OH}	Gln3^{OE1}	H2	H
Tyr55H^{OH}	Asp179^{OD2}	H2	H
Ser58H^{OG}	Asp111^{N}	H2	H
Ser58H^{OG}	His110^{ND1}	H2	H
Tyr60H^{OH}	Asp111^{OD1}	H2	H
Tyr60H^{OH}	Asp111^{OD2}	H2	H
Tyr60H^{OH}	Asp112^{OD1}	H2	H
Tyr60H^{OH}	Asp112^{OD2}	H2	H
Tyr60H^{OH}	Lys100^{NZ}	H2	H
Arg101^{NH1}	Asp228^{O}	H3	H

	Arg101^{NH2}	Asp228^{O}	H3	H
	Arg102^{NH1}	Asp111H^{O}	H3	H
	Arg102^{NH2}	Asp111H^{O}	H3	H
VACV-138				
	Thr28H^{OG1}	Lys48^{Nz}	H1	H
	Asp31H^{OD2}	Thr34^{OG1}	H1	H
	Asp31H^{OD2}	Lys48^{Nz}	H1	S
	Asp31H^{O}	Gln37^{NE2}	H1	H
	Asp31H^{O}	Thr35^{OG1}	H1	H
	Asp52H^{OD2}	Arg44^{NH1}	H2	S
	Asp52H^{OD1}	Arg44^{NH2}	H2	S
	Gln54H^{OE1}	Ser65^{OG}	H2	H
	Gln54H^{NE2}	Asn46^{OD1}	H2	H
	Glu55H^{OE1}	Lys108^{NZ}	H2	S
	Glu55H^{OE2}	Arg44^{NH1}	H2	S
	Glu55H^{OE2}	Tyr104^{OH}	H2	H
	Glu55H^{O}	Lys108^{NZ}	H2	H
	Glu57^{OE1}	Asn175^{ND2}	H2	H
	Thr74H^{OG1}	Glu105^{OE2}	FR	H
	Glu99H^{OE1}	Ser147^{OG}	H3	H
	Glu99H^{OE2}	Ser147^{N}	H3	H
	Tyr98L^{OH}	Asn145^{ND2}	L3	H
VACV-304				
	Asn31H^{OD1}	Asn145^{ND2}	H1	H
	Trp33H^{NE1}	Ser147^{O}	H1	H
	Lys52H^{NZ}	Ser140^{OG}	H2	H
	Gln53H^{NE2}	Ser147^{OG}	H2	H
	Gln53H^{OE1}	Ser147^{N}	H2	H
	Glu102H^{O}	Asn46^{ND2}	H3	H
	Glu102H^{O}	Thr35^{OG1}	H3	H
	Glu102H^{OE1}	Thr34^{OG1}	H3	H
	Ala104H^{N}	Ser147^{OG}	H3	H
	Ser109H^{N}	Glu105^{OE2}	H3	H
	Leu27L^{O}	Lys48^{NZ}	L1	H
	Gln30L^{O}	Lys48^{NZ}	L1	H
	Asp50L^{OD1}	Lys48^{NZ}	L2	S
	Asp50L^{OD2}	Lys48^{NZ}	L2	S
	Ser51L^{OG}	Lys98^{NZ}	L2	H
	Glu52L^{OE1}	Tyr104^{N}	L2	H
	Arg53L^{N}	Ser102^{O}	L2	H

[a] Hydrogen bond (H), salt-bridge (S)

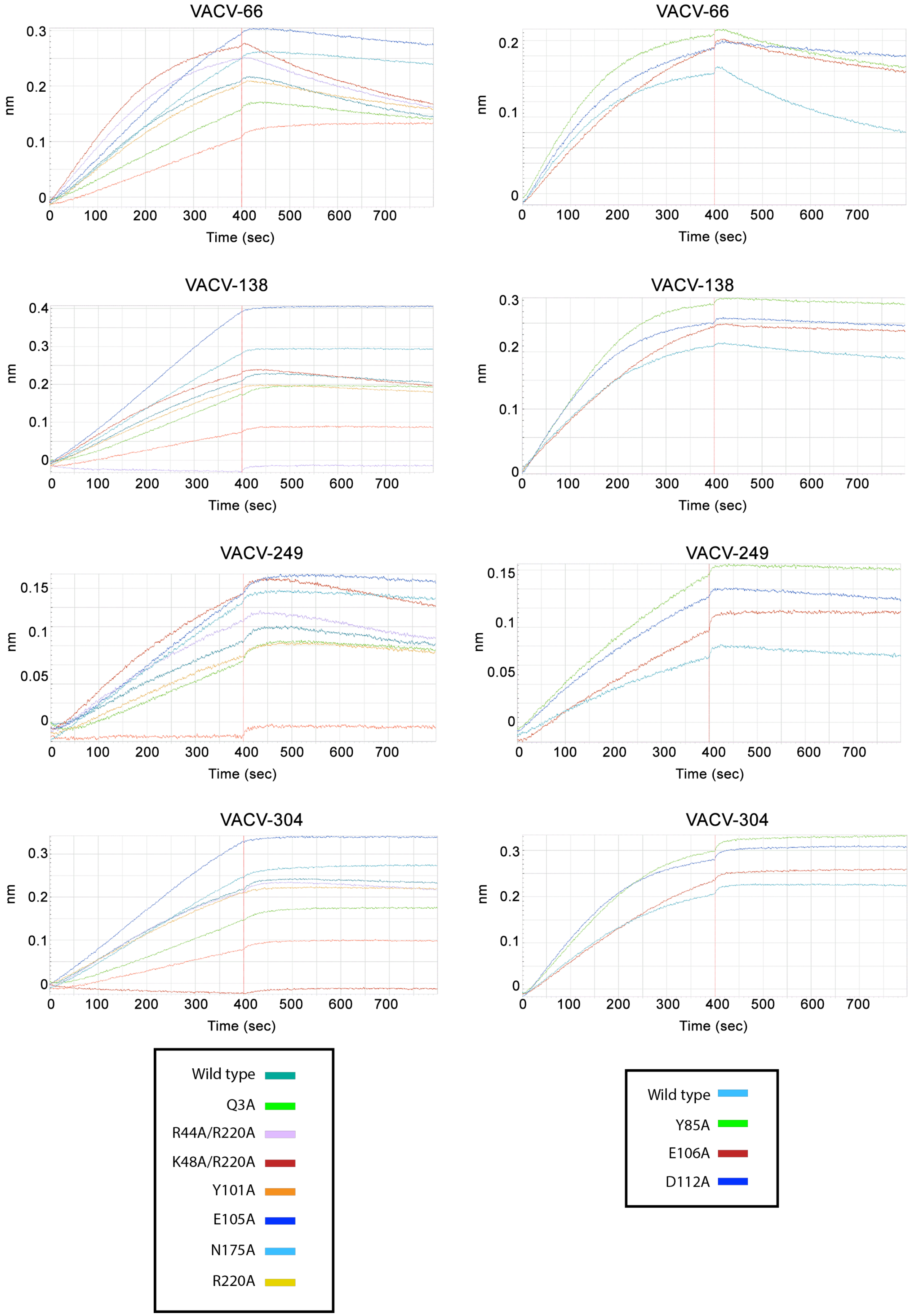

Figure S1. Antibody binding to D8 mutants. BLI experiment using a single dose of indicated MAb to various immobilized D8 mutants.

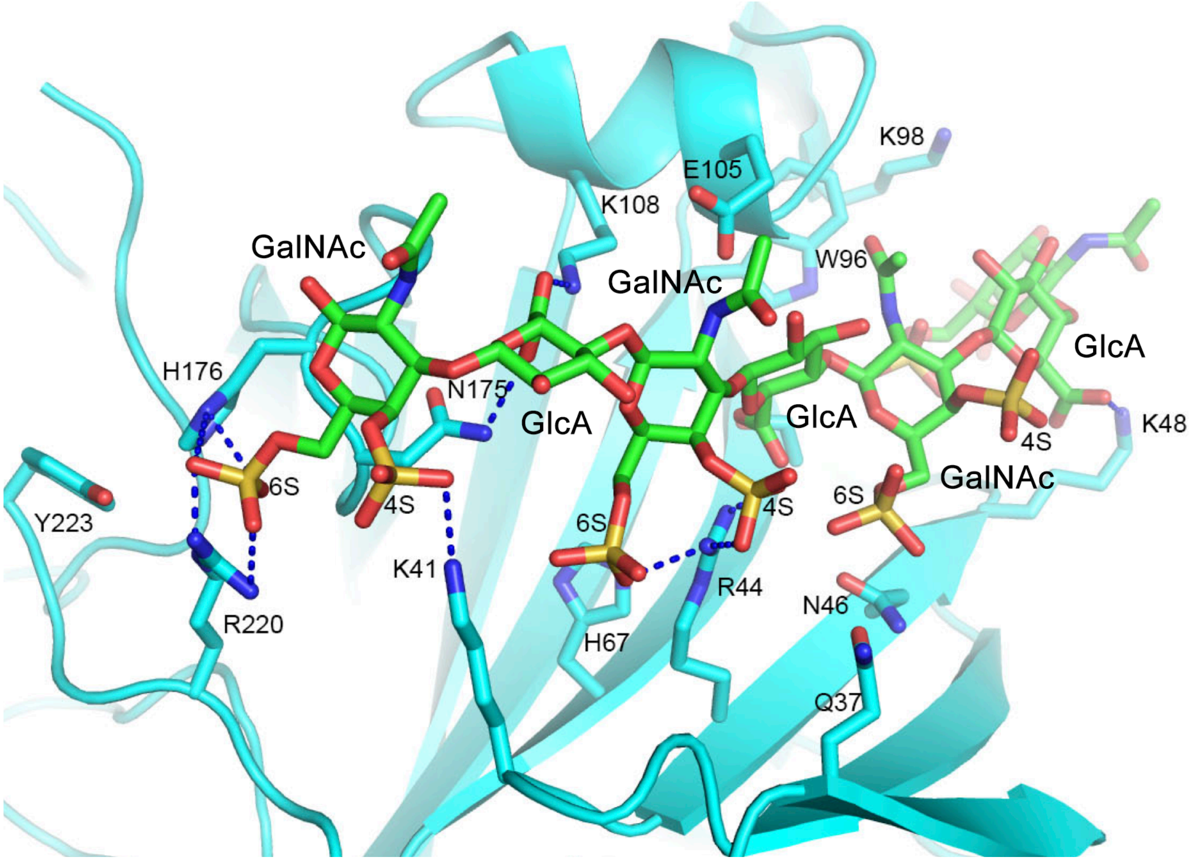

Figure S2. D8-CS-E model. Computational model of CS-E (green sticks) binding along the central crevice of D8 (in cyan), with individual D8 residues indicated. Predicted polar interactions shown as blue dotted lines. GalNAc, N-acetyl galactosamine; GlcA, glucuronic acid.