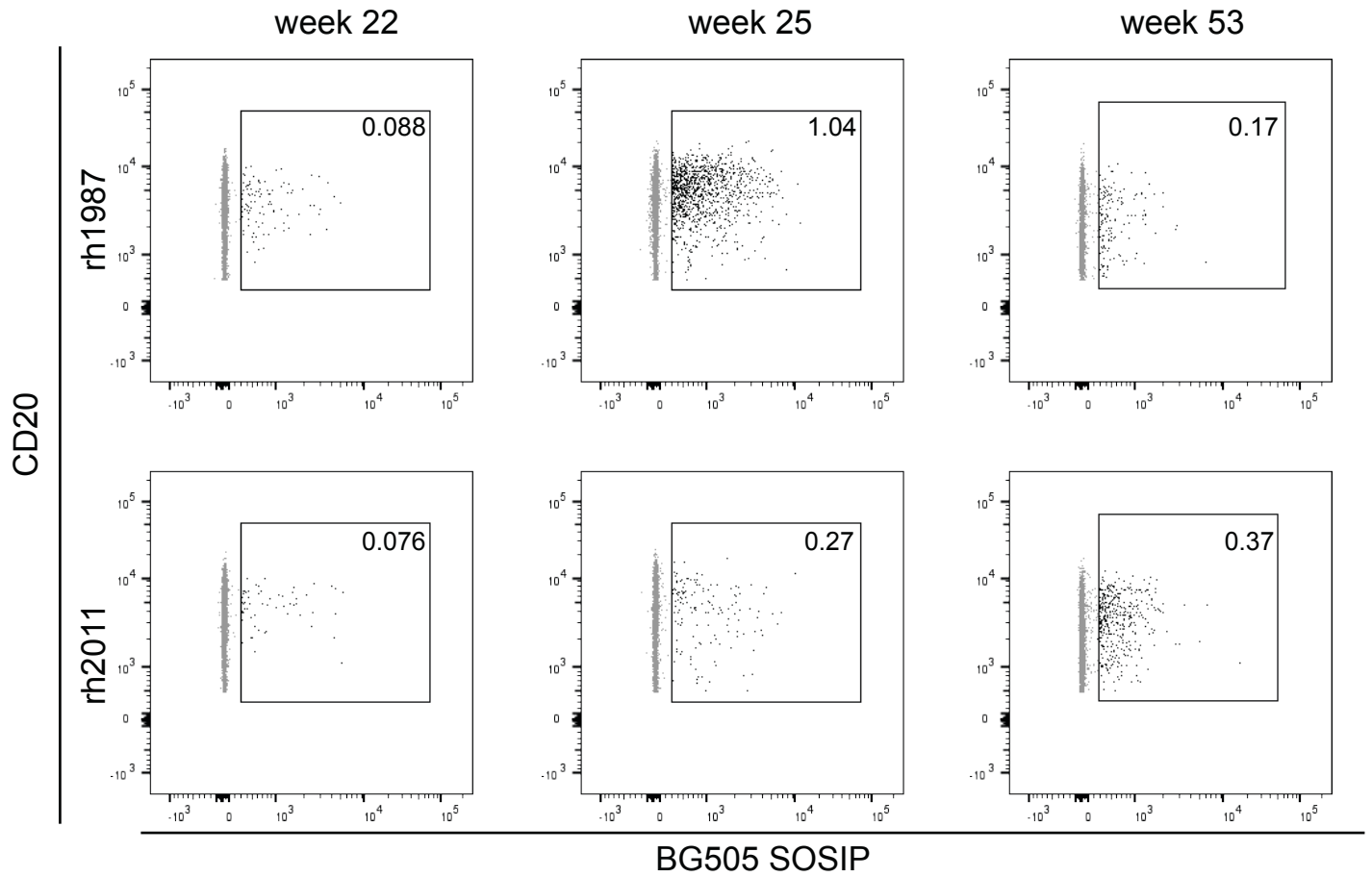


# Supplemental Data

**A**



**B**

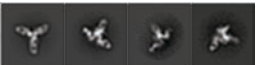





















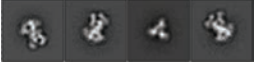

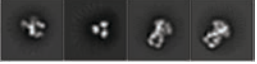



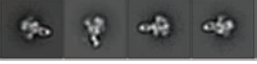

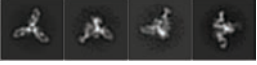







mAb	SOSIP ELISA	gp120 ELISA
RM19A	++	+++
RM19A1	+++	+++
RM19A2	+++	+++
RM19A3	++	+
RM19B	++	-
RM19B1	+	-
RM19C	+	-
RM19C2	++	-
RM19C3	++	-
RM19C4	++	+
RM19D	+++	+++
RM19E	+	-
RM19F	+	-
RM19F1	++	-
RM19G	++	-
RM19J	++	-
RM19K	+++	++
RM19L	++	-
RM19M	++	-
RM19N	+	+
RM19O	+++	+++
RM19P	+++	+++
RM19R	++	-
RM19S	++	-
RM19T	++	++

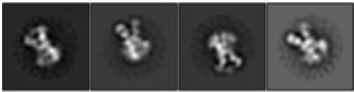














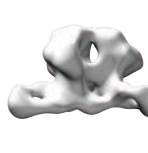






**C**

mAb	SOSIP ELISA	gp120 ELISA
RM20A	++	-
RM20A1	++	-
RM20A2	++	-
RM20A3	++	-
RM20B	+	-
RM20B1	+	-
RM20C	+	-
RM20D	++	+++
RM20E	+++	+
RM20E1	++	+
RM20E2	++	+
RM20E3	+	+
RM20F	++	+
RM20G	++	-
RM20H	++	++
RM20I	++	++
RM20J	+++	+++

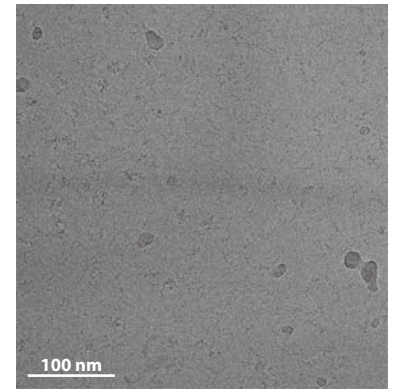
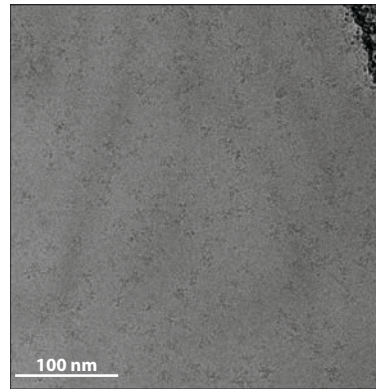
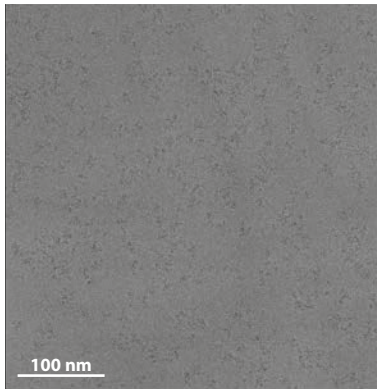
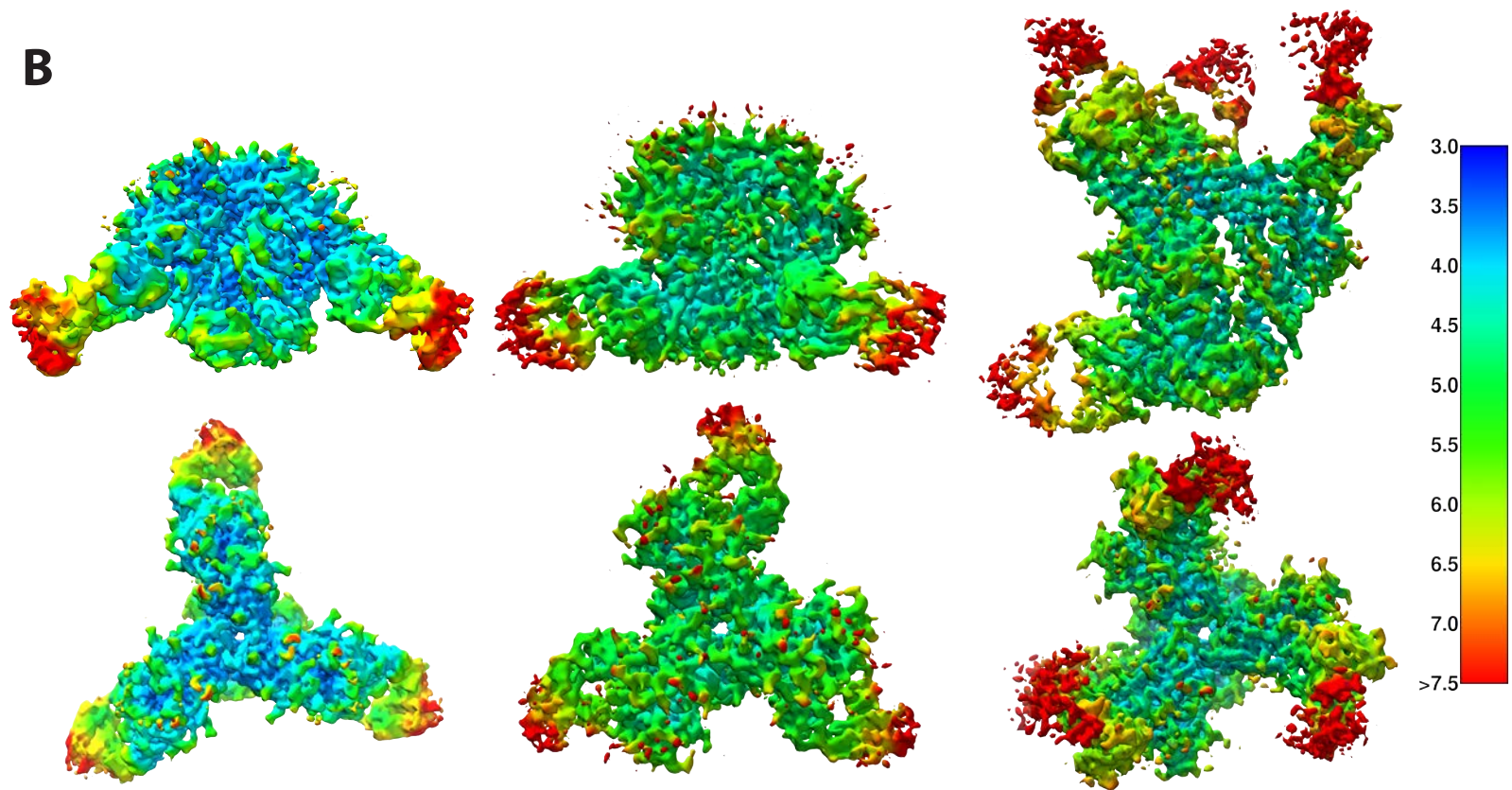
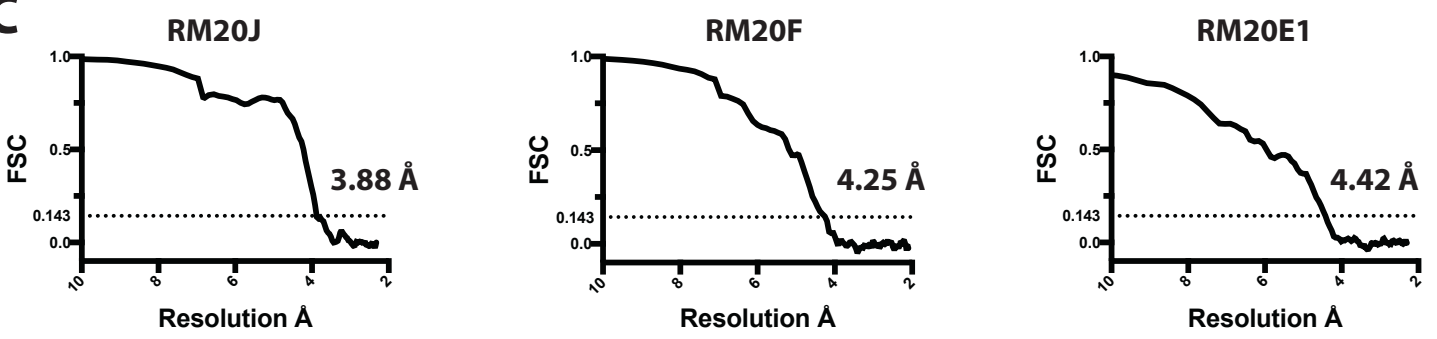
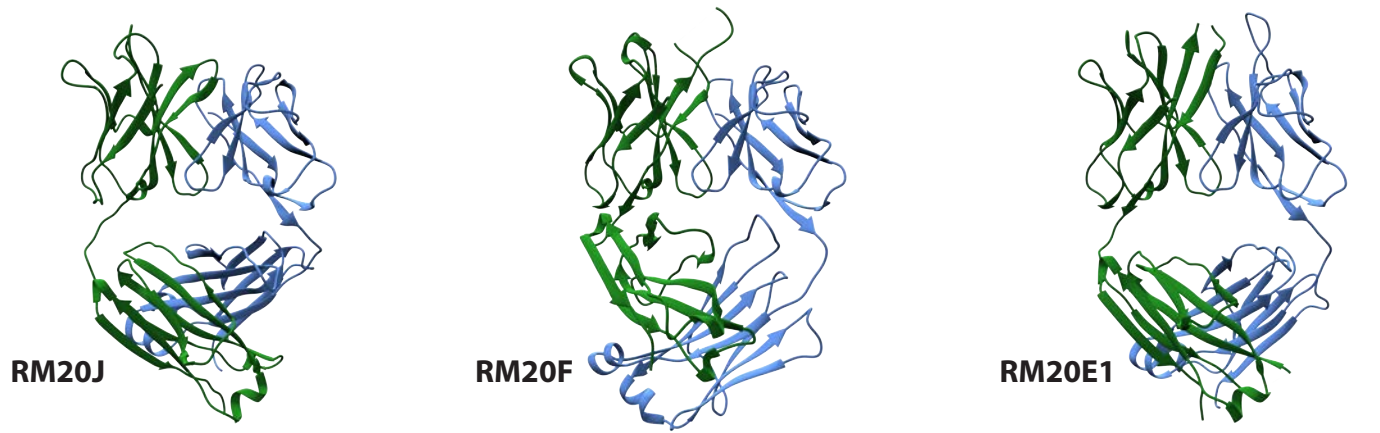
EC50 (ug/mL)	
<0.1	+++
0.1-1	++
1-10	+
>10	-

**Figure S1.** MAb isolation and characterization from BG505 SOSIP.664 trimer-immunized macaques. (A) FACS gating strategy for isolation of BG505 SOSIP specific memory B-cells. (B) BG505 SOSIP.664 trimer and BG505 gp120 ELISA binding data for mAbs isolated from RM rh1987. (C) BG505 SOSIP.664 trimer and BG505 gp120 ELISA binding data for mAbs isolated from RM rh2011.

mAb name	2D class averages	3D reconstructions	Epitope	EMDB#
RM19A1			289 GH	EMD-21062
RM19B			base	EMD-21075
RM19B1			base	EMD-21077
RM19C			base	EMD-21078
RM19C2			base	EMD-21079
RM19C3			base	EMD-21082
RM19E			base	EMD-21080
RM19F			base	EMD-21056
RM19G			base	EMD-21081
RM19J			289 GH	EMD-21055
RM19K			base	EMD-21076
RM19L			base	EMD-21066
RM19M			base	EMD-21061
RM19N			base	EMD-21053
RM19O			base	EMD-21065
RM19P			289 GH	EMD-21064
RM19R			base	EMD-21058
RM19S			N611/FP	EMD-21059
RM19T			N289 GH	EMD-21057

mAb name	2D class averages	3D reconstructions	Epitope	EMDB#
RM20A2			base	EMD-21083
RM20A3			base	EMD-21084
RM20B			base	EMD-21085
RM20B1			base	EMD-21086
RM20C			base	EMD-21087
RM20E			N611/FP	EMD-21093
RM20E1			N611/FP	EMD-21090
RM20F			gp120/gp41 interface	EMD-21091
RM20G			base	EMD-21088
RM20H			gp120/gp41 interface	EMD-21092
RM20J			289 GH	EMD-21089

**Figure S2.** Negative stain electron microscopy epitope mapping of Fabs from rh1987 and rh2011. Representative 2D class averages, 3D reconstructions, and EMDB accession numbers.

**A****B****C****D**

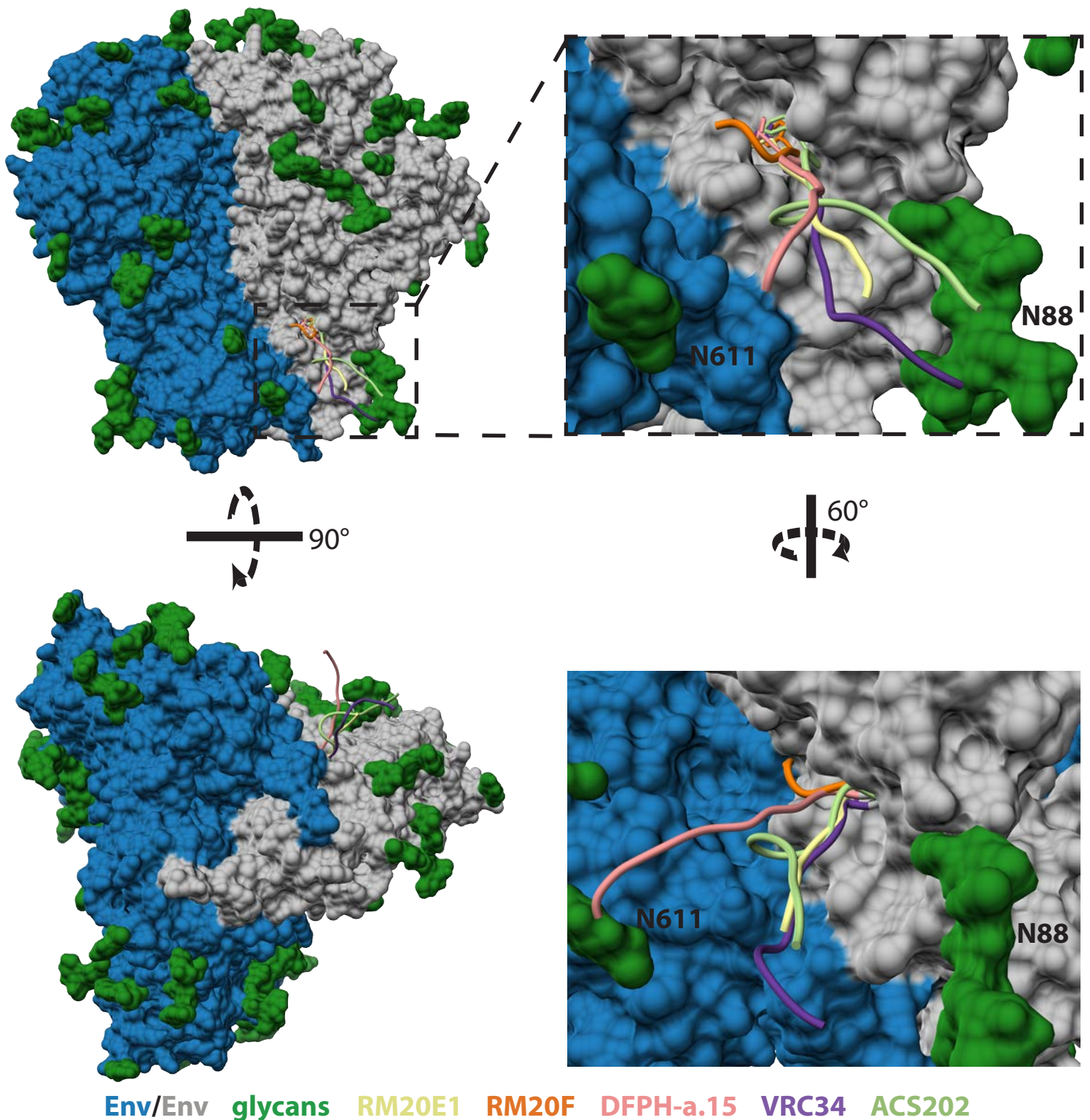
**Figure S3.** Cryo-EM structures of BG505 SOSIP trimers with mAbs and crystal structures of mAbs. (A) Representative micrographs for cryoEM datasets. (B) Local resolution maps for each complex generated in cryoSPARC v2 (Punjani et al., 2017). (C) Gold-standard Fourier shell correlation (FSC) curves for each complex showing global resolution calculated at FSC = 0.143. (D) Crystal structures of unliganded Fabs RM20J, RM20F, and RM20E1. Heavy chains are shown in green and light chains shown in light blue.



Virus name	Tier*	Subtype	Accession	RM20F	ACS202*	VRC34*
001428_2_42	2	C	EF117266	>100	>10	0.075
1012_11_TC21_3257	1B or 2	B	EU289184	>100	>10	n.d.
AC10_29	2	B	AY835446	>100	>10	>10
BJOX010000_06_2	2	01_AE	HM215373	>100	0.506	>10
BJOX015000_11_5	2	01_AE	HM215377	>100	0.023	n.d.
BJOX025000_01_1	2	01_AE	HM215386	>100	0.003	>10
BJOX028000_10_3	2	01_AE	HM215389	>100	0.005	>10
C2101_C1	2	01_AE	JN944661	>100	n.d.	0.218
C3347_C11	2	01_AE	JX512902	>100	>10	>10
C4118_9	2	01_AE	JQ352782	>100	0.411	>10
CAP210_E8	2	C	DQ435683	>100	0.297	0.183
CAP45_G3	2	C	DQ435682	>100	n.d.	0.056
CNE20	2	07_BC	HM215406	>100	>10	>10
CNE5	2	01_AE	HM215415	>100	>10	>10
DU156_12	2	C	DQ411852	>100	n.d.	>10
DU172_17	2	C	DQ411853	>100	n.d.	0.078
PVO_4	2 or 3	B	AY835444	>100	0.043	>10
Q23_17	1B	A1	AF004885	>100	>10	0.099
Q842_D12	2	A1	AF407160	>100	n.d.	0.138
REJO4541_67	2	B	AY835449	>100	>10	>10
RHPA4259_7	2	B	AY835447	>100	0.012	1.559
SC422_8	2	B	AY835441	>100	>10	>10
THRO4156	2	B	AY835448	>100	n.d.	>10
TRJO4551_58	3	B	AY835450	>100	0.029	7.334
TRO_11	2	B	AY835445	>100	>10	>10
ZM109_4	1B or 2	C	AY424138	>100	n.d.	1.432
ZM135_10A	2	C	AY424079	>100	n.d.	>10
ZM197_7	1B or 2	C	DQ388515	>100	n.d.	>10

**Figure S4.** Neutralization data for a panel of 40 heterologous pseudoviruses against RM20F, ACS202, and VRC34. \*Data obtained from Los Alamos National Lab (LANL) CATNAP application (Yoon et al., 2015).





**Figure S5.** Antibody bound FP conformations. The HIV Env trimer is shown as a surface representation with one protomer colored in grey, the other two protomers colored in blue, and the N-linked glycans colored in green. The FP (residues 512-522) from the antibody bound structures of RM20E1, RM20F, DFPH-a.15 (PDB: 6N1W), VRC34 (PDB: 5I8H), and ACS202 (PDB: 6NC2) are shown as colored backbone ribbon diagrams.

Supplementary Table 2. MAb Characteristics

mAb	Timepoint	Animal ID	LC type	VH gene	D gene	JH gene	HCDR3 aa	HCDR3 length	HC %SHM	VL gene	JL gene	LCDR3 aa	LCDR3 Length	LC %SHM	Epitope Targeted
RM19A	week 22	rh1987	Kappa	IGHV3-AFE*01 S3736	IGHD4-22*01	IGHJ4*01	ARGGVYSNYEF	11	4.3%	IGKV1-AAL*01 S2543	IGKJ1-I1	QQVNSYPPT	9	5.3%	289 glycan hole*
RM19A1	week 25	rh1987	Kappa	IGHV3-AFE*01 S3736	IGHD4-22*01	IGHJ4*01	ARGGVYSNYDF	11	6.3%	IGKV1-AAL*01 S2543	IGKJ1-I1	QQVNSDPPT	9	4.4%	289 glycan hole
RM19A2	week 25	rh1987	Kappa	IGHV3-AFE*01 S3736	IGHD4-22*01	IGHJ4*01	ARGGVYSNYDF	11	7.2%	IGKV1-AAL*01 S2543	IGKJ1-I1	QQVNSDPPT	9	5.6%	289 glycan hole*
RM19A3	week 25	rh1987	Kappa	IGHV3-AFE*01 S3736	IGHD4-22*01	IGHJ4*01	ARGGVYSNYDY	11	3.4%	IGKV1-AAL*01 S2543	IGKJ1-I1	QQHNRDPPT	9	4.0%	289 glycan hole*
RM19D	week 22	rh1987	Kappa	LJI.Rh IGHV3.50	IGHD3-26*01	IGHJ6*01	VRDYGGGLD	10	3.3%	IGKV2-ABE*01	IGKJ2-I2	TQGLEFPYS	9	2.6%	n.d.
RM19J	week 25	rh1987	Kappa	IGHV4-AGU*01 S6650	LJI.Rh IGH4.24	IGHJ4*01	ARFNSGDYDF	10	8.6%	IGKV1-AAL*01 S2543	IGKJ3-I3	QHNTYPLT	9	5.6%	289 glycan hole
RM19N	week 25	rh1987	Kappa	IGHV4-S40 S2532	IGHD2-8*01	IGHJ4*01	ARERVVSATSDVYVYFDY	17	2.1%	IGKV1-S57	IGKJ2-I2	QHSYDTPYS	9	4.4%	base
RM19P	week 25	rh1987	Kappa	IGHV4-AGU*01 S6650	IGHD6-29*01	IGHJ4*01	SSSGWSV	7	7.7%	IGKV1-AAY*01	IGKJ2-I2	QQVNSYPYS	9	3.7%	289 glycan hole
RM19R	week 25	rh1987	Kappa	IGHV4-S40 S2532	IGHD3-3*01	IGHJ5-1*01	AFFWSTYYKRFDV	13	8.8%	IGKV3-AAP*01 S6980	IGKJ1-I1	HQENDWPWT	9	6.0%	base
RM19S	week 53	rh1987	Kappa	IGHV4-ABB*01 S8200	IGHD3-9*01	IGHJ4*01	ARRRRYGGDDYGYWRSFYFDS	23	7.4%	LJI.Rh IGKV1.56	IGKJ4-I4	QQDYSTPPT	9	5.3%	N611/FP
RM19T	week 25	rh1987	Kappa	IGHV4-AGU*01 S6650	LJI.Rh IGH4.24	IGHJ4*01	ARFNSDYDF	9	9.5%	IGKV1-AAL*01 S2543	IGKJ3-I3	QHNRYPPT	9	4.4%	289 glycan hole
RM19B	week 22	rh1987	Lambda	IGHV1-AAU*01 S5608	IGHD6-11*01	IGHJ5-2*01	ARIPWRSIAIPMRGNSFDV	20	4.4%	IGLV2-ABJ*01 S3398	IGLJ1-S1	SSYAGNSYTI	10	4.5%	base
RM19B1	week 22	rh1987	Lambda	IGHV1-AAU*01 S5608	IGHD6-11*01	IGHJ5-2*01	ARIMWRSIAIPMRGNSMDV	20	6.7%	IGLV2-ABJ*01 S3398	IGLJ1-S1	SSYAGNSYTI	10	6.0%	base
RM19C	week 22	rh1987	Lambda	IGHV4-AGU*01 S6650	IGHD2-8*01	IGHJ5-2*01	ARYCRGSLCYGGGSLDV	17	7.9%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTLV	10	1.8%	base
RM19C2	week 25	rh1987	Lambda	IGHV4-AGU*01 S6650	IGHD2-8*01	IGHJ5-2*01	ARYCSGSLCYGGGSLDV	17	9.8%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTLV	10	4.3%	base
RM19C3	week 25	rh1987	Lambda	IGHV4-AGU*01 S6650	IGHD2-8*01	IGHJ5-2*01	ARYCSGALCYGGGSLDV	17	7.3%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTLL	10	1.8%	base
RM19C4	week 25	rh1987	Lambda	IGHV4-AGU*01 S6650	IGHD2-8*01	IGHJ5-2*01	ARYCRGSLCYGGGSLDV	17	10.2%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTLV	10	2.7%	base*
RM19E	week 22	rh1987	Lambda	LJI.Rh IGHV3.122 S8388	IGHD2-35*01	LJI.Rh IGHJ5.4	VRVVVSATRGDHFV	15	6.3%	IGLV8-ABK*01	IGLJ6-S6	LIYMGSGISV	10	6.2%	base
RM19F	week 22	rh1987	Lambda	LJI.Rh IGHV4.79.a	IGHD2-35*01	IGHJ4*01	ARFLVVAIKAATVPLEY	18	3.9%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTYVL	11	0.9%	base
RM19F1	week 22	rh1987	Lambda	LJI.Rh IGHV4.79.a	IGHD2-35*01	IGHJ4*01	ARFLVVAIKAATVPLEY	18	5.1%	IGLV2-ABE*01	IGLJ3-S3	SSYAGNSNTYVL	11	0.9%	n.d.
RM19G	week 22	rh1987	Lambda	IGHV1-AAU*02 S1575	IGHD6-6*01	IGHJ4*01	ARDRLAAAGTEHFYD	15	4.2%	LJI.Rh IGLV2.33.a	IGLJ3*01	CSYLSGSTWV	10	3.0%	base
RM19K	week 25	rh1987	Lambda	IGHV1-AAU*01 S5608	IGHD3-26*01	IGHJ5-2*01	ARGLDYGARQLGNSLHV	18	6.1%	LJI.Rh IGLV2.29	IGLJ3*01	YSYAGNSNTW	10	3.0%	base
RM19L	week 25	rh1987	Lambda	LJI.Rh IGHV4.67.a	IGHD2-35*01	IGHJ3*01	ARAPSYGGTSWAFSEGFD	19	6.2%	IGLV11-AAV*01	IGLJ2-S2	QMYGSSGAL	9	3.8%	base
RM19M	week 25	rh1987	Lambda	IGHV4-AGU*01	IGHD3-9*01	LJI.Rh IGHJ5.4	ARDGYENDYGFYHPVHRFDV	21	8.4%	LJI.Rh IGLV2.112	IGLJ3*01	FSYTTNKTWV	10	10.6%	base
RM19O	week 25	rh1987	Lambda	IGHV4-AGR*01	IGHD3-26*01	IGHJ4*01	AAGGGYGNHFD	13	5.9%	IGLV2-ABE*01 S2946	IGLJ1*01	SSYAGNSSTHLF	11	3.1%	base
RM20E	week 53	rh2011	Kappa	IGHV5-ABI*01 S2502	IGHD1-7*01	IGHJ5-1*01	VMWVYILTTGNIWVDV	16	6.4%	LJI.Rh IGKV2.71	IGKJ2-I2	QQITDFPYS	9	3.6%	N611/FP
RM20E1	week 53	rh2011	Kappa	IGHV5-ABI*01 S2502	IGHD1-7*01	IGHJ5-1*01	VMWVYILTTGNIWVDV	16	5.4%	LJI.Rh IGKV2.71	IGKJ2-I2	QQITDFPYS	9	3.6%	N611/FP
RM20E2	week 53	rh2011	Kappa	IGHV5-ABI*01 S2502	IGHD1-7*01	IGHJ5-1*01	VMWVYILTTGNIWVDV	16	5.1%	LJI.Rh IGKV2.71	IGKJ2-I2	QQITDFPYS	9	4.5%	N611/FP*
RM20E3	week 53	rh2011	Kappa	IGHV5-ABI*01 S2502	IGHD1-7*01	IGHJ5-1*01	VMWVYILTTGNIWVDV	16	5.4%	LJI.Rh IGKV2.71	IGKJ2-I2	QQGTFPYS	9	3.0%	N611/FP*
RM20F	week 53	rh2011	Kappa	IGHV3-AFY*10	IGHD3-14*01	IGHJ2-I1	ARGGKPIYSGGYPSWYFDL	20	7.3%	IGKV6-ABK*01	IGKJ3-I3	QQTNSFPCT	9	5.3%	gp120/gp41 interface
RM20H	week 53	rh2011	Kappa	LJI.Rh IGHV3.76.a S4190	IGHD2-13*01	IGHJ5-1*01	AKDWVGDYTYGTYPGWFV	20	6.0%	IGKV3-ADW*01	IGKJ4-I4	QQNSNWPLT	9	4.0%	gp120/gp41 interface
RM20I	week 53	rh2011	Kappa	IGHV4-ACQ*01 S4946	IGHD3-3*01	IGHJ4*01	ARRVSRDLFGGAFDC	15	6.2%	LJI.Rh IGKV2.71.a	IGKJ4-I4	QQGTHWPLT	9	3.9%	n.d.
RM20J	week 53	rh2011	Kappa	IGHV4-AGU*01 S6650	IGHD1-1*01	IGHJ4*01	ARWSTADFDY	10	8.2%	IGKV1-AAL*01 S2543	IGKJ3-I3	QQHNNYPLT	9	5.1%	289 glycan hole
RM20A	week 22	rh2011	Lambda	IGHV3-AFE*01 S3736	IGHD6-29*01	IGHJ4*01	AKGGMSSAWQSSKYYFDF	18	5.3%	IGLV2-ABE*01 S2946	IGLJ1-S1	SSYAGSKTFYI	11	4.2%	base*
RM20A1	week 22	rh2011	Lambda	IGHV3-AFE*01 S3736	IGHD6-29*01	IGHJ4*01	ARGGMSAWQSSKYYFDF	18	8.5%	IGLV2-ABE*01 S2946	IGLJ1-S1	SSYAGRNTFYV	11	6.4%	base*
RM20A2	week 25	rh2011	Lambda	IGHV3-AFE*01 S3736	IGHD6-29*01	IGHJ4*01	ARGGMSAWQSSKYYFDF	18	9.1%	IGLV2-ABE*01 S2946	IGLJ1-S1	SSYAGRNTFYV	11	4.6%	base
RM20A3	week 53	rh2011	Lambda	IGHV3-AFE*01 S3736	IGHD6-29*01	IGHJ4*01	ATGGMSALQSSKYYFDF	18	9.1%	IGLV2-ABE*01 S2946	IGLJ1-S1	SSYAGRQTFYI	11	4.8%	base
RM20B	week 25	rh2011	Lambda	IGHV4-S11	IGHD2-35*01	IGHJ5-1*01	ARLLVSAIRWEDRFV	16	3.0%	LJI.Rh IGLV2.18	IGLJ1-S1	SSLGSGTYI	10	5.1%	base
RM20B1	week 25	rh2011	Lambda	IGHV4-S11	IGHD2-35*01	IGHJ5-1*01	ARLLVSAIRWEDRFV	16	3.8%	LJI.Rh IGLV2.18	IGLJ1-S1	SSFAGGTYI	10	4.7%	base
RM20C	week 25	rh2011	Lambda	IGHV3-AEW*01	IGHD3-9*01	IGHJ4*01	TRVAYEHYGYKYYFDF	20	4.4%	IGLV1-ACV*01	IGLJ6-S6	QSYDSSLSAHV	11	4.5%	base
RM20D	week 25	rh2011	Lambda	IGHV3-AFY*05	IGHD4-15*01	IGHJ4*01	ARDPSRYGNYPDN	13	3.6%	IGLV4-ACF*02	IGLJ3-S3	QWTAGIVS	9	2.1%	n.d.
RM20G	week 53	rh2011	Lambda	IGHV3-AEW*01	LJI.Rh IGH4.29	IGHJ6*01	TRMRFASAQEPVYVYGM	17	6.7%	IGLV1-S16 S2133	IGLJ1-S1	AAWDDSLGGYI	11	3.3%	base

\*Inferred based on clonal relationship to mAbs with epitopes mapped by ns-EM. Clonal families are highlighted with individual colors.

**Supplementary Table 3. BLI Binding Kinetics**

<b>mAb</b>	<b>KD (M)</b>	<b>kon (1/Ms)</b>	<b>kdis (1/s)</b>
RM19A	n.d.	n.d.	n.d.
RM19A1	3.94E-10	1.41E+04	5.57E-06
RM19A2	n.d.	n.d.	n.d.
RM19A3	n.d.	n.d.	n.d.
RM19B	9.87E-10	3.12E+05	3.08E-04
RM19B1	7.00E-10	4.01E+05	2.80E-04
RM19C	1.50E-09	2.66E+05	4.00E-04
RM19C2	<1.0E-12	1.12E+05	<1.0E-07
RM19C3	6.80E-11	9.95E+04	6.76E-06
RM19C4	n.d.	n.d.	n.d.
RM19D	1.57E-07	1.68E+03	2.63E-04
RM19E	1.28E-10	2.80E+05	3.60E-05
RM19F	4.98E-09	6.30E+05	3.14E-03
RM19F1	2.88E-08	7.98E+04	2.30E-03
RM19G	3.95E-07	2.67E+03	1.05E-03
RM19J	1.95E-08	3.98E+03	7.77E-05
RM19K	8.55E-08	3.72E+03	3.18E-04
RM19L	6.03E-10	1.02E+05	6.15E-05
RM19M	1.03E-08	2.27E+04	2.34E-04
RM19N	1.46E-08	3.66E+05	5.33E-03
RM19O	1.87E-08	3.82E+04	7.14E-04
RM19P	2.09E-09	8.26E+03	1.73E-05
RM19R	5.52E-10	1.12E+05	6.18E-05
RM19S	1.47E-07	7.16E+03	1.05E-03
RM19T	8.45E-10	2.28E+04	1.93E-05
RM20A	n.d.	n.d.	n.d.
RM20A1	n.d.	n.d.	n.d.
RM20A2	<1.0E-12	8.95E+05	<1.0E-07
RM20A3	<1.0E-12	7.82E+05	<1.0E-07
RM20B	3.92E-08	1.67E+04	6.56E-04
RM20B1	1.85E-09	3.48E+05	6.44E-04
RM20C	2.55E-09	2.67E+04	6.79E-05
RM20D	n.d.	n.d.	n.d.
RM20E	n.d.	n.d.	n.d.
RM20E1	5.85E-10	5.75E+04	3.36E-05
RM20E2	n.d.	n.d.	n.d.
RM20E3	n.d.	n.d.	n.d.
RM20F	1.60E-08	8.11E+03	1.30E-04
RM20G	8.01E-11	5.71E+05	4.58E-05
RM20H	1.61E-08	1.37E+04	2.21E-04
RM20I	1.27E-07	2.53E+03	3.21E-04
RM20J	<1.0E-12	4.47E+04	<1.0E-07

**Supplementary Table 4. EM Data Collection and Map/Model Refinement Parameters**

Complex	BG505.v4.1 + RM20F	BG505.v5.2 + RM20J	BG505.v5.2 + RM20E1 + PGT122
Microscope	Titan Krios	Talos Arctica	Talos Arctica
Voltage, kV	300	200	200
Detector	Gatan K2 Sumit	Gatan K2 Sumit	Gatan K2 Sumit
Recording Mode	Counting	Counting	Counting
Magnification	29,000	36,000	36,000
Moive micrograph pixel size, Å	1.03	1.15	1.15
Dose rate, e <sup>-</sup> /[(camera pixel)*s]	8.833	6.004	5.656
No. of frames per moive micrograph	24	44	48
Frame exposure time, ms	250	250	250
Movie micrograph exposure time, s	6	11	12
Total dose, e <sup>-</sup> /Å <sup>2</sup>	50.0	49.9	51.3
Defocus range, μm	1.3 to 2.8	1.0 to 3.5	1.0 to 2.5
No. of movie micrographs	1055	553	579
No. of molecular projection images in map	91212	26327	17010
Symmetry	C3	C3	C1
Map resolution (FSC 0.143)	4.25	3.88	4.42
Map sharpening B-factor, Å <sup>2</sup>	-174.7	-112.6	-81.2
No. of atoms in deposited model	19962	19785	21768
MolProbity score	1.16	1.38	0.97
Cβ Outliers (%)	0.00	0.00	0.00
Rotamer Outliers (%)	0.15	0.72	0.13
Rama Outliers (%)	0.65	1.29	0.20
Clashscore	1.75	2.12	0.97
EMRinger score	2.02	2.71	1.82
Privateer	pass	pass	pass
EMDB	EMD-21246	EMD-21257	EMD-21232
PDB ID	6VN0	6VO1	6VLR

**Supplementary Table 5.** X-ray data collection and refinement statistics

Data collection	RM20F (PDB:6VSR)	RM20J (PDB:6VOS)	RM20E1 (PDB:6VOR)
Beamline	SSRL 12-2	APS 23ID-B	SSRL 12-2
Wavelength (Å)	0.97946	1.03322	0.97946
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P 4 <sub>3</sub> 2 <sub>1</sub> 2	P 1
Unit cell parameters	a=61.5, b=75.6, c=115.1, α=β=γ=90	a=b=112.3, c=141.0, α=β=γ=90	a=57.4, b=57.7, c=92.7, α=98.7, β=94.1, γ=97.8
Resolution (Å)	36.7-2.20 (2.24-2.20) <sup>a</sup>	50.0-2.30 (2.34-2.30) <sup>a</sup>	50.0-1.85 (1.90-1.85) <sup>a</sup>
Unique Reflections	28,053 (1,364) <sup>a</sup>	40,057 (1,946) <sup>a</sup>	142,088 (2,413) <sup>a</sup>
Redundancy	4.0 (4.0) <sup>a</sup>	17.5 (11.2) <sup>a</sup>	2.7 (1.3) <sup>a</sup>
Completeness (%)	98.6 (99.4) <sup>a</sup>	100 (99.6) <sup>a</sup>	85.4 (32.5) <sup>a</sup>
$\langle I/\sigma_I \rangle$	7.7 (2.0) <sup>a</sup>	28.0 (1.0) <sup>a</sup>	18.8 (1.2) <sup>a</sup>
$R_{\text{sym}}^b$ (%)	19.7 (83.0) <sup>a</sup>	12.9 (>100) <sup>a</sup>	10.9 (69.1) <sup>a</sup>
$R_{\text{pim}}^b$ (%)	11.0 (46.4) <sup>a</sup>	3.0 (50.3) <sup>a</sup>	4.9 (51.7) <sup>a</sup>
CC <sub>1/2</sub> <sup>c</sup> (%)	83.9 (54.0) <sup>a</sup>	89.7 (44.1) <sup>a</sup>	91.6 (56.0) <sup>a</sup>
<b>Refinement statistics</b>			
Reflections (work)	26,622	39,953	75,965
Reflections (test)	1,374	1,999	3,285
$R_{\text{cryst}}^d / R_{\text{free}}^e$ (%)	19.7/24.1	18.1/21.1	22.4/25.2
No. of atoms			
Protein	3,328	3,604	6,731
Water	288	224	320
Average B-value (Å <sup>2</sup> )			
Protein	25	62	39
Water	34	68	40
Wilson B-value (Å <sup>2</sup> )	21	57	30
<b>RMSD from ideal geometry</b>			
Bond length (Å)	0.002	0.007	0.008
Bond angle (°)	0.55	0.95	0.99
<b>Ramachandran statistics (%)</b>			
Favored	97.5	96.1	96.3
Outliers	0.0	0.2	0.1

<sup>a</sup> Numbers in parentheses refer to the highest resolution shell.

<sup>b</sup>  $R_{\text{sym}} = \frac{\sum_{hkl} \sum_i |I_{hkl,i} - \langle I_{hkl} \rangle|}{\sum_{hkl} \sum_i I_{hkl,i}}$  and  $R_{\text{pim}} = \frac{\sum_{hkl} (1/(n-1))^{1/2} \sum_i |I_{hkl,i} - \langle I_{hkl} \rangle|}{\sum_{hkl} \sum_i I_{hkl,i}}$ , where  $I_{hkl,i}$  is the scaled intensity of the  $i^{\text{th}}$  measurement of reflection  $h, k, l$ ,  $\langle I_{hkl} \rangle$  is the average intensity for that reflection, and  $n$  is the redundancy.

<sup>c</sup> CC<sub>1/2</sub> = Pearson correlation coefficient between two random half datasets.

<sup>d</sup>  $R_{\text{cryst}} = \frac{\sum_{hkl} |F_o - F_c|}{\sum_{hkl} |F_o|} \times 100$ , where  $F_o$  and  $F_c$  are the observed and calculated structure factors, respectively.

<sup>e</sup>  $R_{\text{free}}$  was calculated as for  $R_{\text{cryst}}$ , but on a test set comprising 5% of the data excluded from refinement.