Supplementary Movie Descriptions

sm-1. This movie, produced using Powerpoint, shows the results of classifying simultaneously on all three arms of the Env spike (whole spike classification) as an animated sequence with descriptions. This classification was done prior to superimposing each Env spike arm and computing a classification on one site as is shown in Figure 3. The class averages are shown in red superimposed on the symmetrized average of antibody free arms acting as an unliganded control spike. (A) View down the 3-fold axis of the spike, (B) view obtained by rotating the spike about the horizontal average and away from the observer by 45°, and (C) view tangential to the membrane plane. Numbers below the right hand panel are the number of class members. The three-arm classification shows Ab bound to 3 sites in class 8 (indicated by arrows), two sites in classes 0-2, 6,-7, 9 and one site in classes 3-5.

sm-2. This movie, produced using Powerpoint,, shows the results of classifying over a single spike arm (single gp120) after triplicating each spike and rotating one copy 120° and the other copy 240°, but as an aligned animated sequence with descriptions. (A) View down the 3-fold axis of the spike, (B) view obtained by rotating the spike about the horizontal average and away from the observer by 45°, and (C) view tangential to the membrane plane. Numbers above the right hand panel are the number of class members in the class average. The color coding is identical to that of Figure 3.

sm-3. This movie, produced using Powerpoint, shows the difference density maps of HIV-1 MN Env spike with bound 447-52D antibody shown as an animated sequence with descriptions. Each difference map is superimposed on the "control" unliganded spike. (A) View down the 3-fold axis of the spike, (B) view obtained by rotating the spike about the horizontal average and away from the observer by 45°, and (C) view tangential to the membrane plane. Positive difference map shown in solid color superimposed into the symmetrized, antibody-free density map (in grey solid). The contour threshold displayed is 12x the standard deviation of the density over the entire difference map in order to achieve better localization. This value is between 37% and 47% of the maximum density in the difference map. The coloring scheme is as follows: class01, brick; class02, yellow; class03, cyan; class04, red; class05 magenta; class06, green.

sm-4. This movie produced in Chimera (3), shows morphing of the one-arm class averages together with the atomic models fit to the different class averages using NMFF. The coloring scheme is : Env glycoprotein gp120 core residue 90-124; green, gp120 core residues 198-396 [intact V3 loop has been added to these residues from pdb file 2B4C]; orange, gp120 core residue 410-492; yellow, 447-52D Fab chains red and blue.

sm-5. This movie, produced using Powerpoint, shows the comparison of positive difference maps from HIV/447-52D Env spikes with the soluble, partially deglycosylated spike trimer KNH1144 SOSIP 664G with antibody PGT128 bound, EMDB code EMD-1970 (1). The symmetrized global average of the present work is shown in gray at 50% transparency. These images are shown as an animated sequence with descriptions. Left side column is looking down the axis of the Env spike. Middle column is after rotating the spike about the horizontal axis away from the observer by 45°. Right side column is a view looking tangential to the membrane surface. The difference peaks lie either on the position of the PGT128 Fab or slightly

counterclockwise of it, consistent with motion of the 447D antibody bound V3 loop about a position near its base.

sm-6. This movie, produced using Powerpoint, shows the comparison of the difference maps for the 447-52D class averages with the 3-D reconstruction of PGT135 in complex with the BG505 SOSIP.664 gp140 trimer (2) colored olive (EMDB code emd-2331). The symmetrized global average of the present work is shown in gray at 50% transparency. Coloring for the class average difference peaks is the same as for Figure 3. The orientations shown are, from left to right, down the 3-fold axis, rotated away from the observer by 45°, and tangential to the membrane plane. The difference peaks are generally centered slightly clockwise from the PGT135 Fab, a location that is consistent with the PGT135 antigen being counterclockwise of the base of the V3 loop.

References

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