



Supplementary Figure Side view of the interaction of the CAPS molecule with the CDR-H3.

For crystallization, 100 mM (cyclohexylamino)-1 propanesulfonic acid CAPS buffer, pH 10.5, was used. A well-ordered CAPS buffer molecule was observed bound to CDR-H3 from Fab LH. The six-carbon ring of CAPS nestles into a concave spoon-shaped depression at the top of the CDR H3 loop, and forms specific hydrophobic contacts to Pro H100d, Ser H100c, and Tyr H98. The nitrogen atom in the CAPS stem forms a hydrogen bond to the main-chain carbonyl oxygen of Trp H100. This interaction is of interest as the H3 loop of the antibody is important for recognition of the CD4 binding site on gp120 (11)