2390-2393.), KEK,Japan. The 1.6 Å data set collected at a shorter wavelength of 0.8200 Å yielded a merging R-factor of 0.046 in intensity. After the phase extension and structure refinement subsequent to the molecular replacement analysis, the R-factor for the final model, which contained 233 residues, 155 water molecules and 1 sulfate ion, was 0.178 in the resolution range of 8.0-1.6 Å. The rms deviation of bond lengths for the model was 0.016 Å and the positional error was estimated to be ca. 0.17 Å.

All the complementarity determining region (CDR) loops are clearly visible in the electron density maps. The H3 loop as well as its side chains are well elucidated and can accomodate the dansyl group of the hapten.

The orientation of the VH and VL domains is significantly different from that of McPC603 Fab; when VL domains are superimposed, the angle between the principal axes of the remaining VH domains is 10.7°.

PS–03.03.08 THE STRUCTURE OF HIV-1 NEUTRALIZING ANTIBODY 50.1 By M.Takimoto-Kamimura*+, R. L. Stanfield, E. A. Stura, A. T. Profy and I. A.Wilson, The Department of Molecular Biology, The Scripps Research Institute, La Jolla, U. S. A.

Much evidence suggests that the principle neutralizing determinant of HIV is located in the third variable region(V3) of HIV envelope glycoprotein, gp120 (Bolognesi et al., AIDS , 1989, 3(suppl. 1)., S111-S118; Steimer et al., Science, 1991, 254, 105-108). Antibody 50.1 was derived from mice immunized with a cyclic forty residue synthetic peptide representing the V3 loop of HIV-1 gp120(MN isolate). 50.1 Fab fragment was produced by papain cleavage. Crystals of the free Fab were obtained from high salt in space groups $P2_12_12_1$ and I222 (Stura et al., Proteins , 1992, 14, 499-508). These crystals have been solved at 2.8 Å resolution by the molecular replacement. Similated annealing with X-PLOR gave a model with R factors of 0.19($P2_12_12_1$), 0.20(I222) for the all data between 2.8 to 10.0Å. Different crystal form but conformation similar as indication CDR loops adapt defined conformations not an assembly that is crystal packing dependent. The CDR H1 loop of 50.1 is two residues longer than previously analyzed H1 loop structures. This is a new H1 loop structure. The insertion occurs at the surface loop formed by residues 30 and 31. In addition, the length and sequence of the 50.1 CDR L1 loop is also placed in a new canonical class.

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