Virtual screening of HIV-blocking antagonists: the figure depicts the lowest energy CXCR4/AMD3100 binding conformation identified by AUTODOCK. The view on the left shows AMD3100 docked within the extracellular binding pocket of the CXCR4 receptor, shown as a ribbon cartoon. The AMD3100 molecular volume is depicted using a semitransparent spherical harmonic surface. The view on the right shows in more detail the calculated binding conformation. In this docking prediction, two nitrogens of one AMD3100 cyclam ring interact with the two carboxylic oxygens of Asp262, and two nitrogens of the other cyclam ring interact with the two carboxylic oxygens of Glu288. See V. I. Pérez-Nuño, D. W. Ritchie, O. Rabal, R. Pascual, J. I. Borrell, and J. Teixidó, p 509.