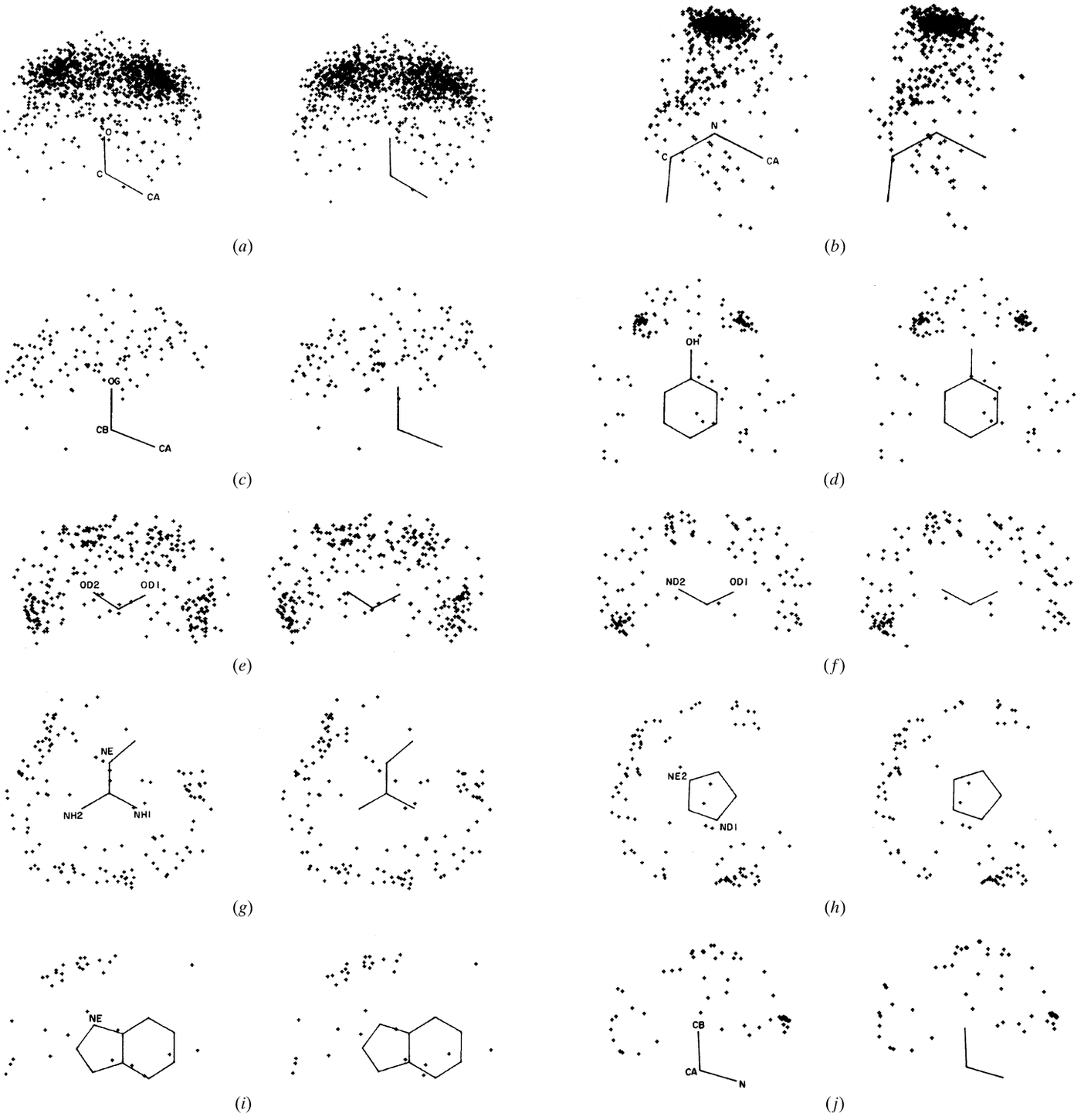

Fig. 23.4.3.1. Distribution of water-molecule sites in stereo around: (*a*) main-chain O, (*b*) main-chain N, (*c*) Ser OG, (*d*) Tyr ring, (*e*) Asp OD1 and OD2, (*f*) Asn OD1 and ND2, (*g*) Arg NH1, NH2 and NE, (*h*) His ring to 3.5 Å, (*i*) Trp ring to 3.5 Å, (*j*) Ala CB. Reprinted with permission from Thanki *et al.* (1988). Copyright (1988) Academic Press.

water molecules that interact with Asn or Gln are involved in hydrogen bonding to both the carbonyl oxygen and the amido nitrogen atoms.

The clustering of water molecules around the planar guanidyl group of Arg is distinctly positioned around the Nε atom and on either side of the NH1 and NH2 atoms. This is shown in Fig. 23.4.3.1(*g*). The clusters peak at a distance of about 3.0 Å from the nitrogen atoms. 7% of these water molecules are shared between NH1 and NH2, and only 3% are shared between the Nε and NH1 atoms. The distribution around the Lys side chain is much broader and is qualitatively similar to the one shown for Ser in Fig. 23.4.3.1(*c*), with no particular orientational preferences, mainly due to the freely rotating nature of the Cε—Nζ bond.

His and Trp are the two residues that contain ring nitrogen atoms, which comprise the main site of interaction with water molecules for these side chains. The distributions of water molecules within 3.5 Å of these residues are shown in Figs. 23.4.3.1(*h*) and (*i*). The clustering around His shows a peak at 2.7 Å and a larger peak at

references