

Supporting Information

Figure Legends

Figure S1. Time dependent variation of dihedral angle $C_{\alpha}-C_{\beta}-C_{\gamma}-C_{\delta 2}$ of His159 in (a) mutant and (b) wild-type papain–substrate, I complexes.

Figure S2. Time dependent variations of (a) $OD1(Asn175)\dots NE2(His159)$, (b) nonbonded angle $OD1(Asn175)\dots NE2(His159)-CG(His159)$ and (c) $OD1(Asp158)\dots ND1(His159)$ in mutant (—) and wild-type (.....) enzyme–substrate, I complexes.

Figure S3. Nonbonded separation between S(Cys25) and nitrile carbon atom, CN versus time in mutant (—) and wild-type (....) papain–peptide nitrile, I complexes.

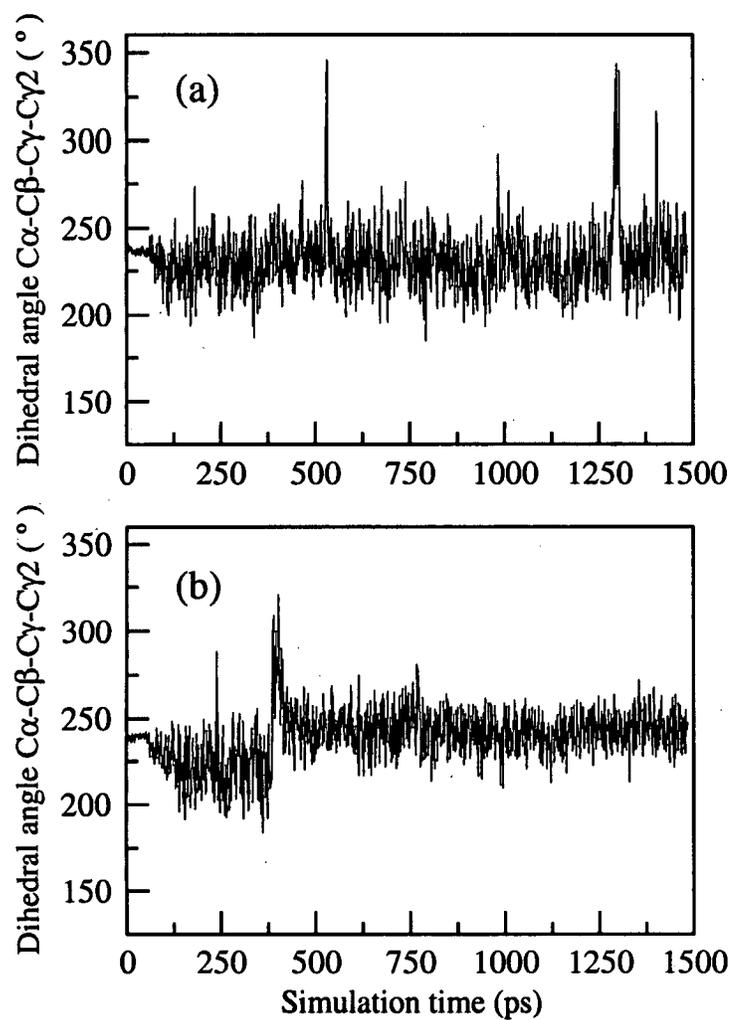


Figure S1

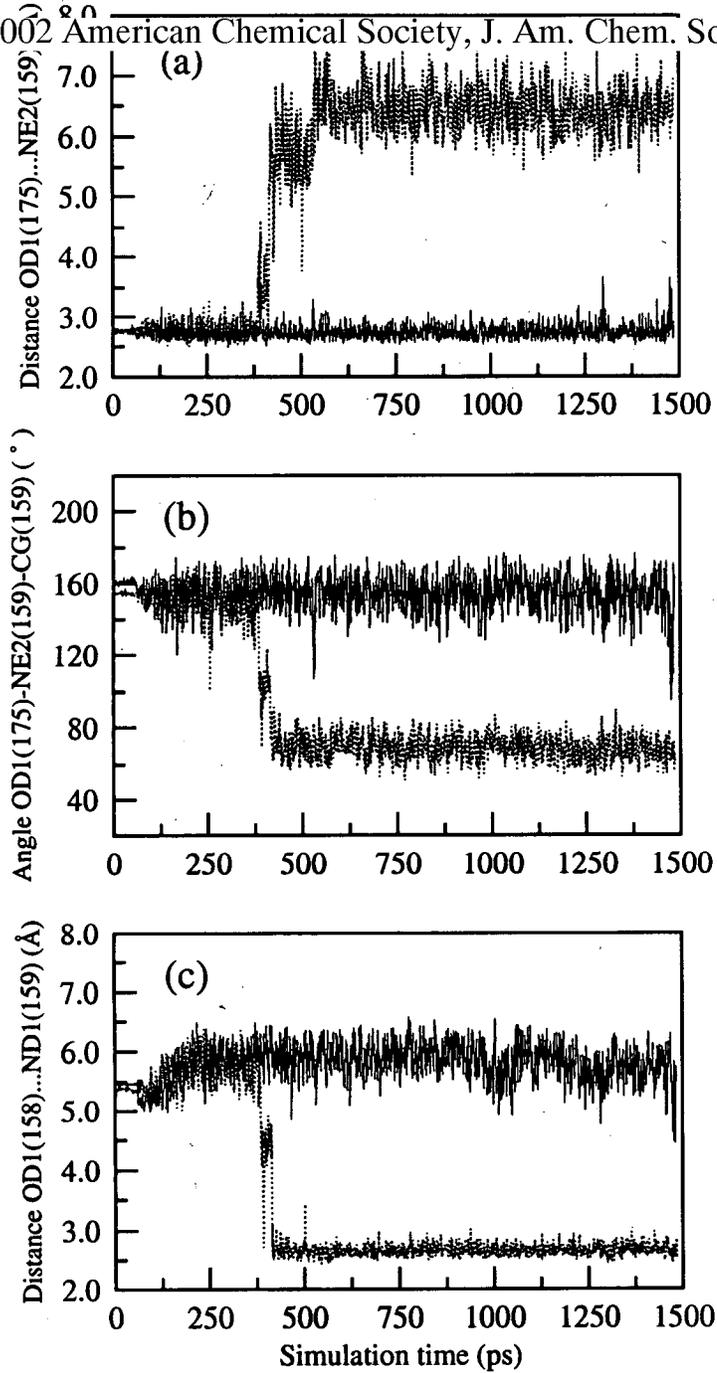


Figure S2

S3

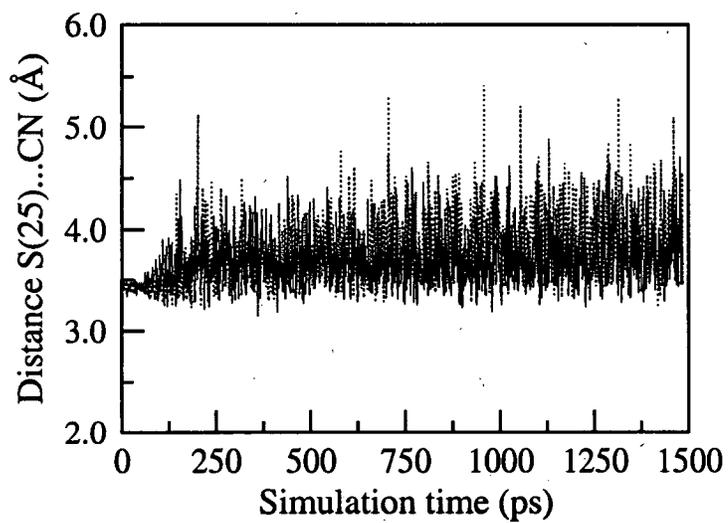


Figure S3

S4