

W0318

Stereochemical Rules for Connecting Disjoint Protein Fragments. Andrzej Kudlicki, Maga Rowicka, Zbyszek Otwinowski, UT Southwestern Medical Center, 5323 Harry Hines Blvd Dallas, TX 75390-9038.

In the process of assembling a protein model, the electron density is fitted with fragments consisting of several peptide units. In low-quality regions of electron density maps, one runs into problems arising from either too many substantially different fragments, or a missing peptide bond. It is then crucial to reduce the set of hypotheses by disqualifying inconsistent ones.

To this end, we characterize the local shape of a main chain segment by angles between vectors connecting four consecutive C-alpha atoms. The local conformation is described by three quasi-conformation angles: two flat and one dihedral angle. We investigate the probability distribution of these angles, and find that the conformation space of the angles is highly restricted. This allows for more efficient connecting of disjoint fragments.

Since the procedure of matching hypotheses is computationally expensive, one needs a simple description of the quasi-conformation angle space. We present such a convenient description, and compute its parameters using data from PDB. Full sets of parameters are provided.