Puck 2, an improved version of the Cremer–Pople puckering program. By Peter Luger and Renate Bülow, Institut für Kristallographie, Freie Universität Berlin, Takustrasse 6, D-1000 Berlin 33, Federal Republic of Germany

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Abstract

The Cremer–Pople ring puckering program has been modified to include the standard deviations of the parameters, calculated from those of the atomic positions, and more convenient input and output.

The Cremer–Pople (1975) puckering parameters provide a general definition to describe the shapes of non-planar n-membered rings. They are widely used for comparing the ring conformations of furanose (n = 5) and pyranose (n = 6) rings in nucleoside and carbohydrate crystal structures (cf. Jeffrey & Sundaralingam, 1981). For n = 5, the two parameters q and q~ can be represented by an angle φ in a circle of radius q. These parameters are closely related to, but not identical (Jeffrey & Taylor, 1980) with the pseudo-rotational diagram of Altona & Sundaralingam (1972). For n = 6, the three parameters q1, θ and φ can be expressed as polar coordinates, thereby providing a convenient graphical representation using the stereographic projection (Jeffrey & Yates, 1979).

The original puckering program (first version written by Jeffrey & Yates, 1979) did not include a calculation of the standard deviations of the puckering parameters from those of the atom coordinates. This was provided later by Taylor.

Fig. 1. Stereographic projection of the conformational sphere (N = 6) as line-printer output. Four six-membered rings were processed, two on the northern hemisphere, marked by a letter N, two on the southern hemisphere, marked S.

Fig. 2. Example of a substituent diagram printed on a line printer. The five-membered-ring data of 1,2,3-tri-O-acetyl-4,5-dideoxy-4-C[(R)-phenylphosphinyl]-α-L-lyxofuranose were used (Luger, Yamamoto & Inokawa, 1982). Various patterns indicate regions of axial, bisectional, equatorial, etc. substituents. Six character atom labels indicate the substituent positions.

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involved in substrate binding. The program is of general use. For example, high-resolution X-ray analyses (Matthews et al., 1981) have been reported for dihydrofolate reductase, inhibitors for which are used in cancer treatment and in the control of bacterial infections.

Quite often the target enzyme itself has not been the subject of an X-ray analysis, but the structure of a closely homologous protein. The three-dimensional structures of several enzymes and other proteins, which are the targets of drugs in wide clinical use. For example, high-resolution X-ray analyses (Matthews et al., 1977; Baker et al., 1981) have been reported for dihydrofolate reductase, inhibitors for which are used in cancer treatment and in the control of bacterial infections. Quite often the target enzyme itself has not been the subject of an X-ray analysis, but the structure of a closely homolo-

**References**


**DOCKER, an interactive program for simulating protein receptor and substrate interactions.** By B. BUSETTA, Laboratoire de Cristallographie et de Physique Cristalline, Université de Bordeaux 1, 351 Cours de la Libération, 33405 Talence, France and I. J. TICKLE and T. L. BLUNDELL, Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HX, England

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**Abstract**

A computer graphics program written for the Evans & Sutherland Picture System 2 allows the interactive docking of a flexible polypeptide into a protein receptor of known three-dimensional structure. Both can be described as either van der Waals or accessible surfaces and a cleft or receptor site can be described as an accessible volume. The program indicates disallowed intermolecular contacts during the docking process, and will also calculate surface-accessible areas and the energy of the system. A non-interactive process of energy refinement can be activated at any time by the user. The program has been used to fit a peptide substrate to the structure of an enzyme, an aspartate proteinase, which has a deep and extended cleft known to be involved in substrate binding. The program is of general value in exploring the complementarity of peptides, which are possible substrates or inhibitors, to proteins whose structures have been defined by X-ray analysis—a process of great importance in rational drug design.

**Introduction**

In the past twenty years X-ray crystallography has defined the three-dimensional structures of several enzymes and other proteins, which are the targets of drugs in wide clinical use. For example, high-resolution X-ray analyses (Matthews et al., 1977; Baker et al., 1981) have been reported for dihydrofolate reductase, inhibitors for which are used in cancer treatment and in the control of bacterial infections. Quite often the target enzyme itself has not been the subject of an X-ray analysis, but the structure of a closely homolo-