s7.m26.p6 **Protein conformer selection by sequence-dependent packing contacts in crystals of 3-phosphoglycerate kinase.** Zoltán Kovári [a,b], Mária Vas [c], [a] *Department of Theoretical Chemistry, Eötvös Loránd University, Budapest, Hungary,* [b] *Department of Computer Assisted Drug Discovery, Gedeon Richter Ltd., Budapest, Hungary,* [c] *Institute of Enzymology, Biological Research Center, Hungarian Academy of Sciences, Budapest, Hungary. E-mail: z.kovari@index.hu*

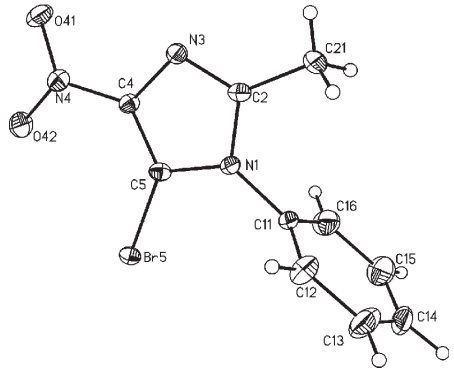
Keywords: Domain conformation; Contact-forming residues; Sequence specificity

In several crystal structures of phosphoglycerate kinase (PGK), the two domains occupy different relative positions. It is intriguing that the two extreme (open and closed) domain conformations have never been observed for the enzyme from the same species. Furthermore, in certain cases, these different crystalline conformations represent the enzyme-ligand complex of the same composition, such as the ternary complex containing either the substrate 3-phosphoglycerate (3-PG) and MgAMP-PNP, an analogue of MgATP; or 3-PG and MgADP. Thus, the domain conformation in the crystal is apparently determined by the origin of the enzyme: PGK from pig muscle has only been crystallized in open conformation, whereas PGK from either *Thermotoga maritima* or *Trypanosoma brucei* has only been reported in closed conformations. A systematic analysis of the sequence differences at the hinge regions and in the crystal contact surfaces, in two independent pairs of open and closed states, have revealed that 1) sequential differences around the hinges do not explain the appearance of fundamentally different conformations and 2) the species-specific *intermolecular* crystal contacts between the nonconserved residues are responsible for stabilizing one conformation over the other in the crystalline state.

s7.m26.p7 **Structural Phase Tranistions in the Crystals of 1-Phenyl-2-methyl-4-nitro-5-bromoimidazole,** Maciej Kubicki, *Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland. E-mail: mkubicki@amu.edu.pl*

Keywords: Phase transitions; Imidazole derivatives; Halogen bonding

The crystals of 1-phenyl-2-methyl-4-nitro-5-bromo-imidazole (1) undergo two reversible phase transitions between 295K and 100K. At room temperature (1) crystallizes in the space group $P2_1/m$ (phase α), the unit cell parameters at 295K: a=7.028(1)Å, b=6.939(1)Å, c=11.561(1)Å, β=106.73(1)°, Z'=1/2 (the molecule occupies the special position: the imidazole ring, methyl, nitro and bromo substituents lie at the mirror plane of symmetry, and the phenyl ring is perpendicular to this plane). The first phase transition, of order-disorder nature, is a second-order transition and takes place continuously over a wide range of temperatures (220 - 170K). This transition is connected with the doubling of c-parameter of the unit cell and with the change of a space group to $P2_1/c$, (phase β) with the unit cell parameters (at 120K): a=6.972(1)Å, b=6.817(1)Å, c=22.900(2)Å, β=106.48(1)°, Z'=1. During this transition the molecule (1) loses the Cs symmetry of the phase α. The α→ß phase transition is testified by the behaviour of the displacement parameters in both models (α and β), and by the diminishing of the superlattice reflections, with l-odd indices, when the temperature rises. The second phase transition (first-order) takes place between 118K and 115K, and is accompanied by the change of the crystal symmetry, to triclinic space group P-1 (phase γ, unit cell parameters at 100K: a=6.965(1), b=6.822(1), c=11.398(2), α=92.68(1)°, β=106.51(1)°, γ=90.28(1)°, Z'=1). This phase transition is accompanied by the twinning of the crystal. Neither the molecular geometry nor the crystal packing shows any dramatic changes during these phase transitions. Halogen bonds C-Br···N and dihalogen interactions Br···Br play a crucial role in determining the crystal packing and compete successfully with other kinds of weak intermolecular interactions. The Br···N distances (2.886(6)Å at 100K - 2.952(2)Å at 295K) are the shortest contacts of this kind found so far; shorter distances were found only in heteromolecular complexes with CBr_4. The geometry of these halogen bonds is typical, almost linear C-Br···N angles, ranging from 162.9(1)° to 163.4(2)° testify for the proposed mechanism of this interaction.



The molecule of (1) at 120K.