cell-cell or cell-extracellular matrix interactions by bidirectional signaling. They are involved in a number of physiological processes such as platelet aggregation, inflammation, tumor metastasis and other diseases. The $\alpha\beta$ heterodimeric glycoproteins are composed from 19 different α subunits and 8 different β subunits [1]. The collagen binding integrin family consists of four collagen receptors that have a common $\beta1$ subunit non-covalently bound either to $\alpha1$, $\alpha2$, $\alpha10$ or $\alpha11$ subunit. They all have a 200 amino acid inserted domain (I-domain) in the N-terminal region of the αsubunit, which is responsible for recognition of the ligand [2]. The αI domain folds into a "Rossman fold", which forms a metal ion-dependent adhesion site, referred to as MIDAS [3].

The crystal structure of $\alpha1$I and $\alpha2$I, and also the complex structure of $\alpha2$I bound to a collagen-like peptide, have been solved [4,5,6]. Comparison of the $\alpha2$I in complex with a collagen-like peptide (open conformation) and $\alpha2$I without ligand (closed conformation) showed that conformational changes occur, when the ligand is bound [6].

We have shown that two peptides, CTRKKHDC and CARKKHDC, bind to $\alpha1$I and competitively inhibit collagen binding. We have modeled the open conformation of $\alpha1$I in complex with a collagen-like peptide and characterized the binding of the ligand and the structural changes that are caused [7]. Our aims are to further study the binding of collagen-like peptides to $\alpha1$I and to characterize the conformational changes that might occur.

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Keywords: integrin, I-domain, collagen-binding

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The Structure of the ParC Subunit of Topoisomerase IV from *Streptococcus pneumoniae*
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Topoisomerases relieve torsional stress in DNA within cells by breaking one or both strands of DNA, then either winding or unwinding the DNA helix, followed by strand closure.

TopoIV (whose subunits are encoded by *ParC* and *ParE*) is a decatenating enzyme that resolves interlinked daughter chromosomes following DNA replication. TopoIV uses a double-strand passage mode as does Gyrase (which controls DNA supercoiling by relieving topological stress arising from the translocation of transcription and replication complexes bound to DNA) by a different mechanism: Gyrase wraps DNA around itself, while TopoIV does not. The difference in DNA-wrapping between Gyrase and Topo IV contributes to their different functional roles within cells.

The ParC subunit of TopoIV has been crystallised in tetragonal and hexagonal forms. Analysis of the tetragonal crystals (diffracted significantly better than hexagonal ones) showed that they were internally twinned. Present in the crystal are two *I222* crystal lattices aligned in opposite directions and forming pseudo 4-fold symmetry.

The structure of ParC subunit was solved by Molecular Replacement using a model build on the basis of the homologous GyrA subunit from *E.coli*[1] (1AB4 deposited in the PDB) as a model. Analysis of packing of the protein molecules in the unit cell shows screw axes || to *c*, going in opposite directions.

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Keywords: topoisomerase IV, ParC, twinning

P.04.01.24
A Proposal to Engineer Protein Crystallization through Metal Ions
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A topic of current interest is engineering surface mutations in order to improve the success rate of protein crystallization. This report explores the possibility of using metal-ion-mediated crystal-packing interactions to facilitate rational design. *Escherichia coli* apo acyl carrier protein was chosen as a test case because of its high content of negatively charged carboxylates suitable for metal binding with moderate affinity. The protein was successfully crystallized in the presence of zinc ions. The crystal structure was determined to 1.1 Å resolution with MAD phasing using anomalous signals from the co-crystallized Zn(II) ions. The case study suggested an integrated strategy for crystallization and structure solution of proteins via engineering surface Asp and Glu mutants, crystallizing them in the presence of metal ions such as Zn(II) and solving the structures using anomalous signals [1].

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Keywords: crystallization, crystal packing, anomalous signals

P.04.01.25
The Crystal Structure of Human CDK7 and Its Protein Recognition Properties
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CDK7, a member of the cyclin-dependent protein kinase family, regulates the activities of other CDKs through phosphorylation on their activation segment and hence contributes to control of the eukaryotic cell cycle. CDK7 also assists in the regulation of transcription as part of the transcription factor TFIIH complex. For maximum activity and stability, CDK7 requires phosphorylation, association with cyclin H, and association with a third protein, MAT1.

We have determined the crystal structure of human CDK7 in complex with ATP at 3 Å resolution. The kinase is in the inactive conformation, similar to that observed for inactive CDK2. The activation segment is phosphorylated at Thr170 and is in a defined conformation that differs from that in phospho-CDK2 and phospho-CDK2/cyclin A. The functional properties of the enzyme against CDK2 and CTD as substrates are characterized through kinase assays. Experiments confirm that CDK7 is not a substrate for kinase-associated phosphatase.

Keywords: cyclin-dependent kinase, cell cycle, structure

P.04.01.26
Novel Vapour Diffusion Method
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We present a new method for the crystallization of biological macromolecules, combining advantages of the vapour diffusion method with advantages of the micro-batch method.

The classic vapour-diffusion, either in its hanging-drop or sitting-drop configuration is still the preferred method by many crystallographers. This is mainly due to its inherent dynamics and the final endpoint of the diffusion. The new method uses a combination of two oils. As in the micro batch method, the total system is protected from evaporation by paraffin oil (first phase). However, the protein/precipitant mixture (fourth phase) is able to equilibrate with a reservoir solution (third phase) via a second layer of oil (second phase), present under the upper layer of paraffin oil. The second oil is not miscible either with the paraffin oil, nor does it interact and influence the properties of both phases three and four. Procedures for