purified from buffalo colostrum. The purified lactotransferrin has been crystallized from a 10% ethanol solution. The crystals are orthorhombic and the space group is $P2_12_12_1$ with unit cell dimensions a = 111.40A, b = 150.80A, c = 158.10A. The asymmetric unit contains three molecules of the protein with a solvent content of about 59%. The crystals were stable in the X-ray beam and diffracted beyond 3.0A resolution. The intensity data upto 3.00A resolution on the native crystals have been collected. The molecular replacement method has been used to determine the structure of the protein using the models of human lactoferrin and rabbit serun transferrin protein. The protein possesses a bilobal structure. Further refinement of the structure is in progress.

PS-03.04.18 CRYSTAL STRUCTURE OF CYTOCHROME c_3 FROM *Desulfovibrio desulfuricans* ATCC 27774.

J. Morais*, C. Frazão, P. M. Matias and M. A. Carrondo

C.T.Q.B., Apartado 127, 2780 Oeiras, Portugal

The three-dimensional X-ray structure of cytochrome c_3 from sulphate-reducing bacteria *Desulfovibrio desulfuricans* ATCC 27774 (Dd 27774) (M.W. 13kDa, 107 residues, 4 heme groups) has been determined by the method of molecular replacement, using as model the refined structure of cytochrome c_3 from *Desulfovibrio vulgaris* Miyazaki F (DvM) (Higuchi *et al.*, J. Mol. Biol., 1984, 172, 109-139), since the two proteins share a 45% sequence homology. The c_3 DvM coordinates were retrieved from the Protein Data Bank.

Crystals of c_3 Dd 27774 were obtained in space group $P6_122$, with cell dimensions a=b=61.8Å and c=109.8Å, Z=12. An X-ray diffraction data set was measured with synchrotron radiation at SRS Daresbury, England, using an Enraf-Nonius FAST area detector diffractometer. The intensity data measurements were carried out with program MADNES. Using programs from CCP4 suite,19328 reflections were merged into 11179 unique (84.8% completeness) in the resolution range 1.75<d<20.0 Å, with $R_{merg}(I) = 5.5\%$.

Cross-rotation and translation functions were performed with ALMN and TFSGEN programs (CCP4 suite), respectively. The packing of the molecules in the unit cell was checked on a CYBER 910/470 graphics workstation with TOM/FRODO.

Rigid body refinement of the model and subsequent refinement using molecular dynamics were performed with XPLOR, achieving an R factor of 25.9%, for data up to 2.3 Å. RESTRAIN least-squares refinement is in progress, the current R factor being 22.5%, for data up to 1.9Å.

PS-03.04.19
CRYSTAL STRUCTURE STUDY OF BAR-HEADED GOOSE OXYHEMOGLOBIN. By Zhang Jian, Hua Ziqian*, Lu Guangying and Gu Xiaocheng, Biology Department, Peking University, Beijing 100871, China.

Bar-headed goose (Anser indicus) is a migratory bird which inhabitates around west china's Qinhai lake. On its migratory flight over Mount Everest it is exposed to ambient pO_2 of about 50mmHg which accounts to 20% of pO_2 at sea level. The determination of its hemoglobin crystal structure may partly elucidate the high altitude respiration mechanism where the air is extremely sparse and also the effect of evolutionary pressure to the protein molecular structure.

Oxyhemoglobin crystals suitable for X- ray analysis were grown from polyethylene glycol(PEG) with average MW.6000, at 4° C, pH6.8. The crystals belong to space group $P4_22_12$. Its unit cell parameters are a=b=81.6A, c=107.3A. There is one ab dimer per asymmetric unit. The intensity data were collected from a single crystal on screenless Weissenberg camera using synchrotron X-ray(Sakabe, N.,J. Appl. Cryst. 1983, 20, 404-407). Total independent reflections were 24807 with upper resolution of 1.8A. Intensity R factor was 4.7.

The hemoglobin of Bar-headed goose has about 70% sequence homology to that of human. So the molecular replacement method was used in structure determination. 2.1A resolution human oxyhemoglobin coordinates was taken as model molecule(Shaanan, B. et al., J. Mol. Bio., 1983, 171, 31- 59). The orientation and position of the molecule in the unit cell were determined with AUTOMR program (Matsuura, Y., J. Appl. Cryst., 1991, 24, 1063-1066). The initial model was rotated about (30, 50, 40) degree (polar angle system). Cross rotation function was calculated using data between 10-4A resolution and pattern cutoff radius 30A. The highest peak appeared at (60.38, 175.73, 260.75) of polar angle system and its translation parameters were (40.8A, 0.0A, 32. 2A) calculated from 12-10A resolution data. Rigid body refinement was carried out with CORELS program, allowing only rotation and translation of molecular dimer. This brought the R-factor to 0.447 between 10-4A resolution. The model after CORELS program was then refined by the simulated annealing method with X-PLOR program(Brunger, A.T.,Science, 1987,235,458-460), the R-factor dropped to 28.9% against data between 8-2A resolution without intervention. The root-mean-square deviation of bond length and bond angle were 0.026A and 4.443 degree respectively for all atoms. The model was checked on the graphics with FRODO program. The hame group area fitted well with the 2Fo- Fc electron density map, while the N-terminal area of the peptide chain fitted relatively poor. Further refinement is under way.

PS-03.04.20 CRYSTAL STRUCTURE ANALYSIS OF HEMOGLOBINS WITH MG-SUBSTITUTED α-HEMES AND EITHER UNLIGANDED OR CO β-HEMES. By S-Y. Park*[1] A. Nakagawa[2], H. Morimoto[1], [1]Department of Biophysical Engineering, Faculty of Engineering Science, Osaka University, Osaka 560, Japan., [2]Photon Factory, KEK, Oho, Tsukuba, Ibaraki 305, Japan.

We have been studying metal substituted hybrid hemoglobins represented as $\alpha_2(M)\beta_2(Fe)$ and $\alpha_2(Fe)\beta_2(M)$, where M denotes metal ions substituted for Fe^{2+}. Depending on the kind of metal ion substituted Fe^{2+}, the subunits change their O_2 affinity from the lowest to the highest of the human hemoglobins (Morimoto et al., *Tanpaku Kakusan Koso*, 1987, 32, 557-565). Thus we can study the interaction between the state of the central ion of heme and the state of the globin moiety by comparing their properties.

