ESRF	**Experiment title:** Arrestin	**Experiment number:** LS1491
Beamline: ID14-4	**Date of experiment:** 270299 – 010399 from: 7 am to: 7 am	**Date of report:** 24-8-99
Shifts: group	**Local contact(s):** Anastassis Perrakis	*Received at ESRF:* - 1 SEP. 1999

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Report:

The time mentioned above has been shared with projects LS1351(=LS1495)/LS1494 (=LS1348)/LS1492/LS1491/

G-coupled receptors are important signalling molecules. Their mode of action is tightly regulated, but when they need to adapt to a extremely large variation in signal, such as the light receptors in the eye rods (rhodopsin) or the β-adrenergic receptors they have a adaptation mechanism that involves phosphorylation by a specific kinase (e.g. rhodopsin kinase) and the subsequent shut-down through binding of arrestin. The crystal structure of bovine arrestin was recently determined to 3.4 A by Granzin *et al.*, 1998. In their crystals they found two conformations. We have obtained a different crystal form of arrestin and we have data to 3.4 A. Molecular replacement shows that the packing is clearly distinct from that found by Granzin *et al.* and that there are differences in the conformation of the N- and C-terminus. Due to the low resolution the molecular replacement solution is not very clear throughout. We wanted to extend our resolution and improve the phasing in order to be able to refine the model.

A number of derivative data sets have been collected using the arrestin crystals. Using difference Fouriers based on the molecular replacement solution heavy atom sites could be identified, but refinement was not possible. The same solution could also be found using

SOLVE, but the map was not interpretable and sites could not be refined. Refinement of the molecular replacement solution was similarly impossible.

Closer inspection of the data showed that they are twinned, a special case, since I222 does not normally show any twinning and the intensity statistics are normal. However, the a and b axis are approximately equal, and the twinning operation is the exchange of these two axes. Recently a 2.8 angstrom resolution structure has appeared in Cell (Hirsch et al., Cell 97, 257-269, 1999). Since our data are twinned as well as lower resolution we have decided not to pursue this any further.

	cell	Reso	Rmerge	I/sigma (last shell)	completeness (last shell)
hgb	91.4 160.4 160.5	3.2	11.9	10.4 (1.5)	99.9% (99.9)
pt1	91.2 160.5 160.9	3.5	9.4	6.5 (1.2)	75.9% (76.8)
pta	91.5 159.8 160.1	3.6	13.6	7.6 (1.6)	96.6% (98.2)