S-SAD EXPERIMENT Details for: BM14U 14-U-45

At a minimum if you can provide the following statistics it would be really useful for us:
YELLOW fields not essential but useful, RED fields need your feedback

Experiment date	02 May 2002-03May 2002
Proposal code (BM14U### or MX###)	BM14U 14-U-45
Unit cell	a=60.34 Å, b=84.33 Å, c=87.06 Å, α =116.20, β=102.52, γ=100.07 degrees
Space group	P1
No. a.a. residues/monomer	397
No. Monomers/AU	3
No. sulphurs/monomer	30
Solvent content	
Disulphide bonds	none
Resolution data collected	1.9
Wavelength used for data collection	0.97950
Data collection strategy (crystal offset, use of kappa etc)	Oscillation ranges for each image ranged between 0.5 and 1.0 degrees with typical exposure times of 1 second per image. Crystal-to-detector distances varied from 130 mm to 250 mm.
Redundancy	4.7
Other anomalous scatterers present (known or unknown at experiment start e.g. maybe you had other metals or ions such as Cd, Cl, Ca etc –or well bound sulphate ions)	none
Software used for location of sulphurs	Twenty out of thirty expected selenium positions were determined using Shake-and-Bake version 2.1. These selenium positions were refined and phases were computed using SOLVE 2.01, resulting in a figure-of-merit of 0.34 at 2.25 Å resolution.
Software used for Refinement of sites/phasing/solvent flattening	A SAD data set was collected at the beamline X06SA at the Swiss Light Source (SLS) in Villigen. This data set was used to solve and refine the structure initially. Later, slightly higher resolution data were collected at the ID14-14 beamline at the ESRF Grenoble. Redundant data sets were collected at the peak wavelength which was determined experimentally by fluorescence scans. Data were integrated and scaled with MOSFLM/SCALA [37, 38] or XDS [39, 40]. Data collection statistics are given in Table 1. Solvent modification was effected with RESOLVE 2.01 [43] and increased the figure-of-merit to 0.58 at 2.05 Å resolution using the SLS data. The resulting electron density map was easily interpretable. Further density modification was carried out using ArpWarp [44] and concomitantly a partial model including sidechains was built

	automatically. The resulting model was completed using O [45]. Refinement was carried out with CNS [46] against the anomalous peak data. Care was taken to partition both Friedel mates either in the test or working set. Anomalous scattering factors for selenium were refined using CNS after the model had reached an R_{free} of 0.28. In the final stages of refinement NCS restrains were removed. This procedure was judged to be valid by the drop in both R and R_{free} by about 1%.
Experiment success /failure	Successful SAD experiment
Citation for work if published	Achim Stocker, Takashi Tomizaki, Clemens Schulze-Briese and Ulrich Baumann (2002): Crystal Structure of the Human Supernatant Protein Factor, *Structure*, 10, 1533–1540.

We are of course very happy if you have the time to provide full data processing/phasing and refinement statistics and any comments /thoughts on the experiment carried out.