ESRF	**Experiment title: Structure determination of nucleic acid motifs using a defined supramolecular scaffold**	**Experiment number:** LS955
Beamline: ID14 3	**Date of experiment:** from: 11/7/'98, 15.00 to: 13/7/'98, 23.00	**Date of report:** August '98
Shifts: 7	**Local contact(s):** Laurence Dumon	*Received at ESRF:*

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Report:

We were extremely pleased with the data for MS2 we collected during this beam time allocation, especially as we were unsure how are crystals would behave at ID1 4 3. It transpired that it was possible to collect a full data set from a single, albeit translated, unfrozen crystal. This was due to both the small beam size (allowing many translations) and the fast readout time of the CCD (previous experience suggests that data quality degrades over time once the crystal has been initially exposed to x-rays even when exposure is not continueing).

Table 1

Crystal	Resolution(Å)	Completeness(%)	R_{merge}(%)	Redundancy	No. xtals
Native	2.8	86.0	20.7	2.4	4
HIV-l TAR	2.8	87.3	19.6	1.4	1
	2.8	55.4	16.3	1.4	1
HIV-2 TAR	2.8	95.1	19.6	4.0	1

Data were collected from crystals soaked with one principal RNA target, the HIV TAR region in complex with a TAT peptide analogue, argininamide. Crystals soaked in two different RNA designs were used, one based on HIV-1 TAR, the other on HIV-2 TAR. In both cases, complete data sets were collected (see Table 1 for statistics) and subsequent analysis shows bound RNA. The maps are currently being interpreted, a portion of the initial $F_{o(capsid+RNA)}$-$F_{o(capsid)}$ density for the HIV-2 TAR is shown in Figure 1. Data were also collected for unsoaked crystals, this data set allows us to increase the resolution at which we can calculate initial difference density maps as our previous native data set was only useful to 3.5Å.

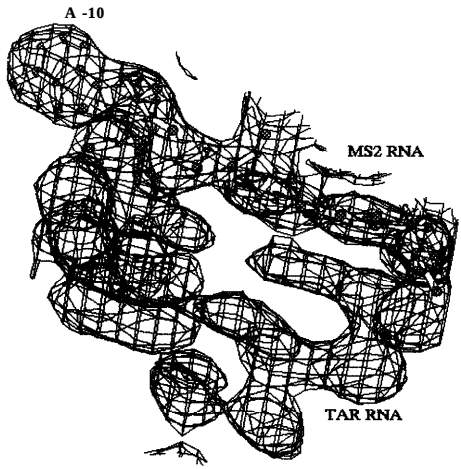

Figure 1

We did not know in advance how the MS2 crystals would behave at ID14 3, therefore we brought crystals of T7 Endonuclease protein to be tested. When this was done, diffraction to 2.0 Å was unexpectedly apparent. Two native data sets were collected at different resolutions (only the lower resolution set has currently been processed) and two putative derivative data sets. The data processing statistics are in Table 2 and work is currently ongoing to locate the heavy atom positions.

Table 2

Crystal	Resolution(A)	Completeness(%)	R_{merge}(%)	Redundancy
Native	2.65	99.4	4.6	4.0
Hg	3.7	85.5	12.5	3.1
Pt	3.0	99.9	15.1	3.8