Summary of data collection on FMDV 3C at BM14 (4-4-04)

Sole aim was to collect multiwavelength data on SeMet-labelled FMDV 3C crystals

Crystal data:
Spacegroup: H3
Cell param: a=144.16 Å b=144.16 Å c=5.19 Å $\alpha = \beta = 90.0$ $\gamma = 120.0$
No. molecules/au = 2
No of anomalous centres per molecule: 11

Useable data obtained from 3 crystals:

Crystal	Energy (keV)	Resolution (Å)	R_{merge} (%)	R_{anom} (%)	Completeness (%)	Multiplicity (%)
x1	12.66195	2.7	8.5 (41.0)	7.0 (19.3)	99.9	9.2
	12.65901	2.7	7.6 (39.8)	7.0 (36.1)	99.7	3.7
	14.00000	2.7	8.3 (41.8)	7.0 (38.7)	99.5	3.6
x2	12.66195	2.0	6.9 (39.0)	5.3 (15.3)	100.0	9.5
	14.00000	1.9	5.0 (37.1)	4.7 (31.8)	99.6	3.1
x3	14.00000	2.0	6.2 (36.5)	5.6 (32.7)	99.7	3.1

x2 gave best data overall (despite 17% merihedral twinning). Se sites detected with SHELXD, refined using SHARP. Map calculated at 1.9 Å looks very clear. Model building and refinement in progress.