



	Experiment title Llama VHH fragments	Experiment number: BAG. LS1508
Beamline: ID14-EH2	Date of experiment: from: 16.11.99 to: 19.11.1999	Date of report: 29.2.2000
Shifts: 1	Local contact(s): MITCHELL Eddy	<i>Received at ESRF:</i>

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Report:

Protein name: VHH CARB24 anti carbazol
 Size: 12.000 Daltons, 120 aa

.Data collection of unliganded VHH CARB24
 Crystals were frozen to 100K, without cryoprotectant. The crystals belong to the space group P3212, with dimensions a=48.2 A, b=48.5 A c=163.9 A alpha=beta=90 gamma=120.000. Two data set were collected to 100K, one to high resolution with an exposure time of 2 s per 0.5 degree and the other to low resolution with an 2 s each 2 degree see table below. Structure solution with MR is underway

Total number of observation	189333
number of unique reflections	28590
overall % data > 1sigma (last shell)	96.7(96.7)
overall R-merge (%) (last shell)	4.5(11.4)
overall I/sigma(I) (last shell)	8.3 (6.3)
resolution	29.0-1.6 A

FV fragments

Protein name: Hybrid scFv fragment where de VL domain of the p185-HER2 binding 4D5 scFV was linked with the VH domain of the levan binding cysteinen-restored A48cys scFV with 2 stabilizing mutations H K66R and II-N52S.

Size: 25.000 daltons

.Data collection of hybrid scFv fragment

Crystals were frozen to 100K, using 30% glycerol. The space group and unit cell dimensions were confirmed from a preliminary exposure to be P3121, a=88.05 Å, b=88.05 Å c=118.4 Å. A data set were collected to 100K, with an exposure time of 2 s per degree, see table below. The 3_D structure of the scFV was determined by molecular replacement. The model is refined with CNS, slow cooling and energy minimisation.

Total number of observation	332476
number of unique reflections	31908
overall % data > 1sigma (last shell)	90.4(90.4)
overall R-merge (%) (last shell)	3.6(27.0)
overall I/sigma(I) (last shell)	13.3(2.7)
resolution	20.0-2.0 Å

Protein name: complex scFV anti-GCN4 binder,
which binds with very high affinity against an unstructured
peptide

Size: 25.000 daltons

.Data collection

Crystals of the complex scFV-peptide were frozen without cryoprotectant. These crystals were of the space group P21 with cell dimensions a=84.0 Å, b=35.96 Å, c= 74.0, beta= 94.54A data set were collected to 100K, with an exposure time of 2 s per degree, see table below. The 3_D structure of the scFV was determined by molecular replacement, using as the search model the same scFV unliganded. The refinement is in progress.

Total number of observation	181241
number of unique reflections	55227
overall % data > 1sigma (last shell)	90.0(89.3)
overall R-merge (%) (last shell)	7.5(23.8)
overall I/sigma(I) (last shell)	4.5(2.4)
resolution	29.0-1.6 Å