
BEAM-LINE: ID29

18-19 Feb 02

3shifts

Project/Protein Name: PA Sm1 + RNA

Principal Investigator: Suck

Experimenters: Thore

Unit Cell Dimensions (Å): 68, 68, 84.5 105 109 100

Space Group: P1

Status of Project: structure solved, paper submitted

	Ligand
Wavelength	0.979
Observations	127088
Unique	34307
Resolution	2.75
Rsym	5.7
Completeness	98.5
I/σ	16.5
Multiplicity	3.7

Project/Protein Name: Exportin complex

Principal Investigator: Conti

Experimenters: Fukuhara, Conti

Unit Cell Dimensions (Å): 115, 145, 280, 90 90 90

Space Group: I222

Status of Project: crystal improvement

	Native
Wavelength	0.979
Observations	16670
Unique	3500
Resolution	7.4
Rsym	9 (24)
Completeness	98.7 (98.6)
I/σ	6 (3)
Multiplicity	4.7 (4.8)

Project/Protein Name: NF1/Sec14

Principal Investigator: Scheffzek

Experimenters: D'angelo

Unit Cell Dimensions (Å): 120 120 100, 90 90 120

Space Group: P622

Status of Project: Looking for phases – no obvious sites from the anomalous of the most promising derivatives

	Au soak	KePtCl ₄ soak	EMP soak
Wavelength	0.934	0.934	0.934
Observations	78820	42750	68820
Unique	5828	3729	5439
Resolution	3.4	4	4
Rsym	7.1	9.7	9.1
Completeness	100	100	99.8
I/ σ	2.0	2.2	2
Multiplicity	13	11.7	7.1

BEAM-LINE: ID14-EH1 6-7 April 01

Project/Protein Name: TAP

Principal Investigator: Conti

Experimenters: Fribourg

Unit Cell Dimensions (Å): 48 81 83

Space Group: P212121

Status of Project: Native collected – complete and at the highest resolution so far. MR so far unsuccessful – preparing for MAD

	Native
Wavelength	0.934
Observations	85967
Unique	6556
Resolution	3.1
Rsym	9.7 (39)
Completeness	97.4 (91)
I/ σ	5.4
Multiplicity	

Project/Protein Name: Exportin

Principal Investigator: Conti

Experimenters: Fernandez

Unit Cell Dimensions (Å): 161 11 121

Space Group: P21212 or P2221

Status of Project: Native data sets collected (new crystal form) – search for heavy atom derivatives/Semet crystallization in progress

	Native 1	Native 2
Wavelength	0.934	0.934
Observations	87128	80363
Unique	18507	21088
Resolution	4	3.6
Rsym	11.4 (41)	13.5 (40.4)
Completeness	99.5 (99.2)	88.4 (75.7)
I/σ	4.5 (1.8)	4.4 (1.8)
Multiplicity	4.7 (4.4)	3.8 (3.7)

Project/Protein Name: Hfq
 Principal Investigator: Suck
 Experimenters: Sauter, Basquin
 Unit Cell Dimensions (Å): 61, 61, 53, 82.6, 87.3 60
 Space Group: P1
 Status of Project: structure solved, refinement in progress

	Native
Wavelength	0.934
Observations	53759
Unique	14455
Resolution	2.9
Rsym	7.8
Completeness	97.4
I/σ	12
Multiplicity	3.7

Project/Protein Name: AP Sm1
 Principal Investigator: Suck
 Experimenters: Sauter, Basquin
 Unit Cell Dimensions (Å): 44, 44, 28.2, 90 90 120
 Space Group: P3
 Status of Project: still twinned

	Native
Wavelength	0.934
Observations	32057
Unique	3344
Resolution	2.15
Rsym	5.6
Completeness	100

I/σ	28.5
Multiplicity	9.6

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7-8 April 02

2 shifts

Project/Protein Name: TAP

Principal Investigator: Conti

Experimenters: Fribourg

Unit Cell Dimensions (Å): 48, 80, 83

Space Group: P212121

Status of Project: SAD and MAD on Se collected – severe crystal decay, no solution found

	Peak (SAD Se)
Wavelength	0.9792
Unique	4193
Resolution	3.6
Rsym	12.8 (31.6)
Completeness	98.7 (99.5)
I/σ	1.6 (0.6)

	Peak (MAD Se)	Infl	Rem
Wavelength	0.9792	0.9793	0.9083
Observations	40176	37390	31104
Unique	2841	2464	1876
Resolution	3.5	3.8	4.1
Rsym	13.1 (31.7)	12.6 (32.4)	12.7 (34.8)
Completeness	97.3 (98.5)	97.7 (98.4)	97.3 (99)
I/σ	3.3 (1.7)	3.4 (1.7)	3.4
Multiplicity	5.4	4.7	4.6

BEAM-LINE: ID14-EH2

3-4 May

Project/Protein Name: SynGAP

Principal Investigator: Scheffzek

Experimenters: Marquez, Gemeinhardt

Unit Cell Dimensions (Å): 110, 110, 83, 90, 90, 120

Space Group: P6

Status of Project: initial measurements. Screening for higher resolution

	Native
Wavelength	0.933
Observations	5055
Unique	925
Resolution	7
Rsym	8.1
Completeness	97.9
I/ σ	12.1
Multiplicity	5.4

Project/Protein Name: Enzyme 1
Principal Investigator: Scheffzek
Experimenters: Marquez, Gemeinhardt
Unit Cell Dimensions (Å): 171, 47, 86, 90, 101, 90
Space Group: C2
Status of Project: preparing for SeMet and heavy atom derivatives

	Native
Wavelength	0.933
Observations	91914
Unique	26527
Resolution	2.4
Rsym	6.5
Completeness	99.5
I/ σ	11
Multiplicity	3.4

Project/Protein Name: Cbb3
Principal Investigator: Scheffzek
Experimenters: Marquez, Gemeinhardt
Unit Cell Dimensions (Å): 186, 88, 126, 90, 95, 90
Space Group: C2
Status of Project: best crystal form so far

	Native
Wavelength	0.933
Observations	
Unique	
Resolution	4.5
Rsym	
Completeness	
I/ σ	

Multiplicity	
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BEAM-LINE: ID14-EH4 19-20 jun 02 4 shifts

Project/Protein Name:
Principal Investigator: Conti
Experimenters: Fribourg, Conti
Unit Cell Dimensions (Å): 48 84 84
Space Group: P212121
Status of Project: MAD data recorded – few Se sites found –phases need to be improved – derivative search in progress

	Peak 3 (Se MAD)	Infl 3	Rem 3
Wavelength	0.9792	0.9795	0.9393
Observations	23629	22862	22963
Unique	6951	6752	5111
Resolution	2.9	3	3.15
Rsym	4.8 (22.2)	5.2 (16.9)	7.8 (31.4)
Completeness	87.1 (87.1)	93.6 (93.6)	94.2 (95.5)
I/σ	3.4 (3.1)	3.4 (3.2)	3.4 (3.5)
Multiplicity	6.7 (3.5)	6.3 (4.6)	6.7 (2.4)

Project/Protein Name: Exportin
Principal Investigator: Conti
Experimenters: Fernandez, Conti
Unit Cell Dimensions (Å): 162 114 122
Space Group: P21212 or P2221
Status of Project: looking for Se sites – ambiguity of the space group

	Peak 1 (Se MAD)	Infl 1	Rem 1
Wavelength	0.9792	0.9795	0.9393
Observations	98366	76200	51697
Unique	28361	22088	14710
Resolution	3.5	3.8	4.2
Rsym	9.6 (37.4)	10.9 (37.6)	14.6 (38.4)
Completeness	99.7 (100)	99.6 (100)	98.4 (99.3)
I/σ	6.4 (1.7)	4.3 (1.8)	4 (1.7)
Multiplicity	3.5 (3.6)	3.4 (3.5)	3.5 (3.5)

	Peak 2 (Se MAD)	Infl 2	Rem 2
Wavelength	0.9792	0.9795	0.9393
Observations	75635	75668	72839
Unique	21922	21934	21796
Resolution	3.8	3.8	3.8

Rsym	7.8 (32.4)	8.0 (38.4)	9.4 (41.3)
Completeness	99.6 (100)	99.6 (100)	99.6 (100)
I/σ	6.5 (2.3)	6.3 (1.9)	4.5 (1.8)
Multiplicity	3.5 (3.5)	3.5 (3.5)	3.5 (3.5)

	Peak 3 (Se SAD)	Native 4	Native 5
Wavelength	0.9792	0.9393	0.9792
Observations	112318	60820	134153
Unique	15604	14887	26830
Resolution	4.3	4.3	3.6
Rsym	14.5 (36.7)	13.6 (37.7)	13.4 (46.2)
Completeness	99.5 (100)	99.3 (100)	99.7 (100)
I/σ	4.4 (2)	4.8 (1.9)	4.5 (1.5)
Multiplicity	7.2 (7.4)	4.1 (4.1)	5 (5)

Project/Protein Name: Y14 complex (EJC)
Principal Investigator: Conti
Experimenters: Fribourg
Unit Cell Dimensions (Å): 140, 140, 68
Space Group: I4
Status of Project: Native data set collected (new crystal form)

	Native
Wavelength	0.9792
Observations	104735
Unique	23227
Resolution	2.5
Rsym	6.5 (26)
Completeness	99.9 (100)
I/σ	4.5 (4.5)
Multiplicity	8.5 (2.8)

Project/Protein Name: NF1/Sec14 Drosophila
Principal Investigator: Scheffzek
Experimenters: D'angelo
Unit Cell Dimensions (Å): 87, 120, 138, 90 90 90
Space Group: P212121
Status of Project: crystallized from a different species where enough methionines for Semet MAD to be feasible

	Native	Native
Wavelength	0.939	0.939
Observations	120392	112494

Unique	19044	13452
Resolution	3.5	3.5
Rsym	8.8	7.9
Completeness	100	100
I/ σ	1.8	2
Multiplicity	6.3	5.9

Project/Protein Name: Inv Inhib
Principal Investigator: Scheffzek
Experimenters: Marquez
Unit Cell Dimensions (Å): 61, 106, 56, 90, 90, 90
Space Group: C222
Status of Project: Preparing for SeMet and heavy atom derivatives

	Native
Wavelength	0.9393
Observations	99415
Unique	15039
Resolution	1.87
Rsym	8.1
Completeness	97
I/ σ	14.9
Multiplicity	6.6

Project/Protein Name: Enzyme 1
Principal Investigator: Scheffzek
Experimenters: Marquez
Unit Cell Dimensions (Å): 171, 47, 86, 90, 101, 90
Space Group: C2
Status of Project: Preparing for SeMet and heavy atom derivatives

	Native
Wavelength	0.9393
Observations	18370
Unique	7837
Resolution	2.6
Rsym	6.3
Completeness	37.3
I/ σ	9.1
Multiplicity	2.3

BEAM-LINE: ID14-EH2 10-11 jul 02 (+ 3shifts on EH1)

Project/Protein Name: Exportin

Principal Investigator: Conti

Experimenters: Fernandez, Conti

Unit Cell Dimensions (Å): 114, 122, 162

Space Group: P21212

Status of Project: one Hg derivative found, space group now unambiguous, heavy atom occupancy + resolution of this derivative to be optimized, planned search for different derivatives

	Hg1	Hg2	Os1
Wavelength	0.933	0.933	0.933
Observations	94864	84731	63511
Unique	19815	21283	15960
Resolution	4	3.9	4.3
Rsym	10.2 (38.1)	9.8 (37.2)	12.2 (42.7)
Completeness	99.8 (99.9)	99.8 (99.9)	99.7 (99.7)
I/σ	5.9 (1.9)	6.7 (1.9)	5.6 (1.7)
Multiplicity	4.8 (4.9)	4.0 (4.1)	4.0 (4.1)

	Ligand 1	Ligand 2
Wavelength	0.933	0.933
Observations	111777	101686
Unique	19795	17737
Resolution	4	4.1
Rsym	10.1 (36.2)	12.3 (38.8)
Completeness	99.7 (100)	97.9 (97.9)
I/σ	5.7 (1.9)	5.3 (2.0)
Multiplicity	5.6 (5.8)	5.7 (5.8)

Project/Protein Name: TAP

Principal Investigator: Conti

Experimenters: Fernandez, Conti

Unit Cell Dimensions (Å): 48, 80, 83

Space Group: P212121

Status of Project: isomorphous Hg derivative found. phases still not enough. Planned a MAD on Mercury and search for other derivatives in progress.

	Native	Hg
Wavelength	0.933	0.933

Observations	18848	17379
Unique	5308	4707
Resolution	3.3	3.45
Rsym	10.4 (33.1)	12.9 (32.9)
Completeness	99.9 (100)	95.9 (94.8)
I/ σ	6.9 (2.2)	5.1 (2.2)
Multiplicity	3.6 (3.7)	3.7 (3.7)

Project/Protein Name: Y14 (EJC)

Principal Investigator: Conti

Experimenters: Fernandez, Conti

Unit Cell Dimensions (Å): 140, 140, 68.5

Space Group: I4

Status of Project: second native collected. Heavy atom search and Semet crystallization in progress.

	Native 2
Wavelength	0.933
Observations	94863
Unique	23022
Resolution	2.5
Rsym	5.5 (32.6)
Completeness	99.4 (99.1)
I/ σ	10.7 (2.3)
Multiplicity	4.2 (4.1)

Project/Protein Name: Enzyme 1

Principal Investigator: Scheffzek

Experimenters: Marquez

Unit Cell Dimensions (Å): 171 47 86 90 101 90

Space Group: C2

Status of Project:

	Native
Wavelength	0.933
Observations	140702
Unique	18508
Resolution	2.7
Rsym	8.1
Completeness	98.4
I/ σ	16
Multiplicity	7.4

Project/Protein Name: Abl-pep
Principal Investigator: Scheffzek
Experimenters: Marquez
Unit Cell Dimensions (Å): 42, 64, 64, 68, 80, 85
Space Group: P1
Status of Project: Structure solved, ligand not bound or only low occupancy. Searching for new crystallization conditions.

	Ligand
Wavelength	0.933
Observations	225197
Unique	49677
Resolution	1.85
Rsym	8.5
Completeness	96.3
I/ σ	11.1
Multiplicity	4.5

Project/Protein Name: Pop
Principal Investigator: Suck
Experimenters: Thore
Unit Cell Dimensions (Å): 77, 77, 101, 90 90 90
Space Group: P41/3
Status of Project: First native data set collected, new project, planning for MAD / MIR

Wavelength	0.933
Observations	63126
Unique	6964
Resolution	3.6
Rsym	9.5
Completeness	100
I/ σ	16.4
Multiplicity	9