ESRF	**Experiment title:** Complexes of threonine synthase	**Experiment number**: LS1794
Beamline: **ID14-EH3**	**Date of experiment**: from: 16-11-00 to: 17-11-00	**Date of report**: 10-2-01
Shifts: 3	**Local contact(s)**: E. GORDON	*Received at ESRF:*

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Report:

The structure of apo-threonine synthase was solved last year using SeMet MAD data collected on BM14. We are now seeking to solve the complex with its activator AdoMet. Two data sets were collected from 2 crystals.

Data collection details : wavelength 0.929Å, distance 170 mm, detector MarCCD, exposure time 40s/ 1degree, 200 degrees measured.

Crystal size about 150x100x50 microns.

The first one was processed with denzo and scaled with scalepack. It gave good data to 2.5Å resolution.

Shell Lower limit	Upper limit	I/Sigma in resolution shells: % of reflections with I / Sigma less than 0	1	2	3	5	10	20	>20	total
30.00	5.38	0.9	2.9	5.5	8.3	13.9	26.1	61.5	37.8	99.3
5.38	4.27	0.6	2.0	3.7	5.7	10.6	22.1	68.4	30.8	99.2
4.27	3.73	0.7	2.1	3.8	5.8	10.7	22.7	56.1	42.7	98.8
3.73	3.39	0.4	1.9	4.7	7.9	14.3	29.4	63.5	35.3	98.8
3.39	3.15	1.1	3.4	7.2	11.6	20.1	39.9	74.9	23.7	98.6
3.15	2.96	1.8	6.3	11.5	16.2	26.4	47.6	82.8	15.9	98.7
2.96	2.82	2.6	7.5	14.6	21.6	34.5	56.5	89.6	8.8	98.4
2.82	2.69	3.6	10.8	19.0	26.6	40.2	63.6	92.7	5.6	98.3
2.69	2.59	5.1	13.5	22.9	31.8	46.0	69.8	95.2	3.0	98.2
2.59	2.50	5.3	14.5	26.0	35.8	50.9	74.7	96.4	1.9	98.2
All hkl		2.2	6.5	11.9	17.1	26.8	45.2	78.1	20.5	98.7

Shell limit	Lower Angstrom	Upper	Average I	Average error	Average stat.	Norm. Chi**2	Linear R-fac	Square R-fac
30.00	5.38		2470.5	139.5	116.0	0.821	0.038	0.062
5.38	4.27		2719.1	157.5	118.9	0.764	0.038	0.069
4.27	3.73		2772.6	149.1	121.6	0.938	0.042	0.062
3.73	3.39		2027.8	114.2	94.6	0.953	0.045	0.057
3.39	3.15		1315.2	86.4	74.8	0.963	0.054	0.063
3.15	2.96		902.5	68.6	61.3	0.915	0.064	0.071
2.96	2.82		634.8	58.1	53.5	0.890	0.078	0.087
2.82	2.69		500.4	53.0	49.8	0.852	0.089	0.087
2.69	2.59		389.8	49.6	47.4	0.834	0.107	0.153
2.59	2.50		332.7	49.0	47.3	0.838	0.123	0.136
All reflections			1409.9	92.6	78.6	0.877	0.050	0.065

The second crystal diffracted to at least 2.2 Å. The data collection details are the same as above with an exposure time 60s/degree and crystal to detector distance of 150mm.
The second data set was processed with mosflm and scaled with scala.

N	1/d^2	Dmin(A)	Rfac	Rfull	Rcum	Ranom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	FRCBIAS	Nbias
$$															
1	0.0205	6.99	0.030	0.041	0.030	0.000	12786.	705.3	18.1	885.	19.7	1516	758	-0.030	299
2	0.0409	4.94	0.035	0.036	0.033	0.000	10062.	660.7	15.2	702.	18.9	3720	1860	-0.062	772
3	0.0614	4.04	0.037	0.041	0.035	0.000	14199.	1014.0	14.0	1033.	18.7	5022	2511	-0.061	1072
4	0.0819	3.49	0.044	0.052	0.038	0.000	10492.	878.9	11.9	780.	17.7	6232	3116	-0.063	1334
5	0.1023	3.13	0.056	0.061	0.041	0.000	6031.	679.5	8.9	487.	15.2	7146	3573	-0.083	1493
6	0.1228	2.85	0.076	0.086	0.045	0.000	3267.	555.7	5.9	312.	12.5	8096	4048	-0.069	1765
7	0.1433	2.64	0.093	0.104	0.048	0.000	2010.	378.8	5.3	251.	9.8	8836	4418	-0.081	1868
8	0.1638	2.47	0.118	0.127	0.051	0.000	1399.	337.5	4.1	229.	7.8	9598	4799	-0.086	2101
9	0.1842	2.33	0.153	0.163	0.054	0.000	946.	288.6	3.3	215.	5.8	10196	5098	-0.100	2172
10	0.2047	2.21	0.188	0.199	0.056	0.000	709.	243.7	2.9	212.	3.8	5306	2653	-0.090	1077
$$															
Overall:			0.056	0.064	0.056	0.000	4685.	574.6	8.2	422.	11.2	65668	32834	-0.067	13953

		Rfac	Rfull	Rcum	Ranom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	FRCBIAS	Nbias

N	1/resol^2	Dmin	Nmeas	Nref	%poss	Cm%poss	Mlplcty	AnomFrc	Rmeas	Rmeas0	(Rsym)	PCV	PCV0
$$													
$$													
1	0.020	6.99	1996	1238	88.1	88.1	1.6	0.0	0.043	0.043	0.030	0.044	0.044
2	0.041	4.94	4365	2505	97.5	94.2	1.7	0.0	0.049	0.049	0.035	0.051	0.051
3	0.061	4.04	5780	3269	98.3	96.0	1.8	0.0	0.053	0.053	0.037	0.055	0.055
4	0.082	3.49	6992	3876	98.4	96.9	1.8	0.0	0.062	0.062	0.044	0.065	0.065
5	0.102	3.13	7948	4375	97.9	97.2	1.8	0.0	0.079	0.079	0.056	0.084	0.084
6	0.123	2.85	8899	4851	98.2	97.4	1.8	0.0	0.107	0.107	0.076	0.114	0.114
7	0.143	2.64	9690	5272	98.1	97.6	1.8	0.0	0.131	0.131	0.093	0.143	0.143
8	0.164	2.47	10443	5644	97.8	97.6	1.9	0.0	0.166	0.166	0.118	0.184	0.184
9	0.184	2.33	11076	5978	97.3	97.6	1.9	0.0	0.216	0.216	0.153	0.240	0.240
10	0.205	2.21	8693	6040	93.0	96.9	1.4	0.0	0.266	0.266	0.188	0.298	0.298
$$													
Overall			75882	43048	96.9	96.9	1.8	0.0	0.079	0.079	0.056	0.084	0.084

			Nmeas	Nref	%poss	Cm%poss	Mlplcty	l	Rmeas	Rmeas0	(Rsym)	PCV	PCV0

An electron density map was calculated for each data set after performing molecular replacement for the second one, and the apoenzyme we know already was present in both. We are currently seeking new conditions to crystallise the complex.