



	<b>Experiment title:</b>	<b>Experiment number:</b> LS2094
<b>Beamline:</b> ID 29	<b>Date of experiment:</b> from: 13-02-02 to: 14-02-02	<b>Date of report:</b> 26/7/02
<b>Shifts:</b> 3	<b>Local contact(s):</b> Bill SHEPHARD	<i>Received at ESRF:</i>
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## Report:

One MAD data set of of the Oxygen Evolving Enhancer complex protein 3 (OEE3) at 2.6 Angstrom resolution have been measured. The protein contains a Zn ion per protein molecule, so a wavelength corresponding to the Zn edge (1.2822 A) was used for the peak, of 1.2827 A for the inflection point and of 0.9189 for the far wavelength

Statistics of the three data sets are as follows:

## Peak:

N 1/d<sup>2</sup> Dmin(A) Rfac Rfull Rcum Ranom Nanom Av\_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS

1	0.0174	7.59	0.050	0.079	0.050	0.058	70	13052.	1053.1	12.4	786.274	433	109	42	-0.123	146
2	0.0347	5.37	0.062	0.073	0.058	0.071	234	8170.	824.4	9.9	533.28.0	1475	299	70	-0.124	590
3	0.0521	4.38	0.069	0.065	0.065	0.050	332	12896.	1381.0	9.3	846.28.4	1982	385	69	-0.100	931
4	0.0694	3.79	0.081	0.085	0.071	0.052	396	10177.	1349.2	7.5	708.26.5	2367	455	76	-0.077	1005
5	0.0868	3.39	0.095	0.090	0.075	0.060	469	5673.	837.5	6.8	466.21.4	2754	524	71	-0.035	1211
6	0.1042	3.10	0.120	0.097	0.079	0.085	527	2523.	485.7	5.2	314.14.7	3091	585	72	0.008	1447
7	0.1215	2.87	0.145	0.095	0.083	0.098	570	1557.	349.3	4.5	292.10.2	3362	642	75	0.070	1562
8	0.1389	2.68	0.196	0.126	0.086	0.142	625	816.	254.3	3.2	283.5.8	3589	696	76	0.070	1765
9	0.1562	2.53	0.243	0.152	0.088	0.198	621	480.	186.3	2.6	279.3.2	3066	622	61	0.053	1353

10 0.1736 2.40 0.331 0.129 0.090 0.298 473 288. 167.7 1.7 281. 1.6 1889 443 38 0.104 562

Overall: 0.090 0.084 0.090 0.066 4317 4205. 736.8 5.7 421. 13.7 24008 4760 650 -0.063 10572  
Rfac Rfull Rcum Ranom Nanom Av\_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS Nbias

**Inflection point:**

N	1/d <sup>2</sup>	Dmin(A)	Rfac	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias
1	0.0137	8.54	0.044	0.088	0.044	0.028	74	25054.	2176.7	11.5	1396.	38.1	863	156	83	-0.094	320
2	0.0274	6.04	0.056	0.060	0.051	0.033	170	14223.	2004.8	7.1	854.	43.6	2144	257	88	-0.121	1043
3	0.0412	4.93	0.070	0.064	0.057	0.038	228	7692.	842.1	9.1	574.	39.1	2906	313	85	-0.081	1679
4	0.0549	4.27	0.072	0.064	0.063	0.029	279	12533.	1442.0	8.7	862.	40.7	3495	374	95	-0.067	2124
5	0.0686	3.82	0.087	0.079	0.068	0.033	326	9028.	1194.6	7.6	744.	37.8	4027	413	87	-0.064	2489
6	0.0823	3.49	0.105	0.083	0.073	0.036	365	5767.	906.3	6.4	645.	31.2	4468	450	85	-0.031	2809
7	0.0960	3.23	0.144	0.113	0.078	0.052	394	2708.	577.3	4.7	557.	23.0	4843	484	90	-0.002	3243
8	0.1097	3.02	0.199	0.136	0.084	0.064	434	1665.	500.8	3.3	562.	16.7	5297	525	91	-0.031	3434
9	0.1235	2.85	0.269	0.210	0.089	0.075	463	1138.	468.9	2.4	578.	12.7	5579	548	85	0.010	3568
10	0.1372	2.70	0.404	0.305	0.095	0.108	488	676.	437.0	1.5	597.	8.1	5856	578	90	-0.025	3937

Overall: 0.095 0.089 0.095 0.037 3221 5386. 964.7 5.6 658. 25.8 39478 4098 879 -0.061 24646  
Rfac Rfull Rcum Ranom Nanom Av\_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS Nbias

**far wavelegth:**

N	1/d <sup>2</sup>	Dmin(A)	Rfac	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias
1	0.0189	7.27	0.050	0.051	0.050	0.000	0	13096.	1076.2	12.2	716.	29.2	447	118	46	-0.098	162
2	0.0378	5.14	0.062	0.061	0.059	0.000	0	8476.	845.0	10.0	495.	32.4	1765	356	82	-0.139	632
3	0.0567	4.20	0.068	0.047	0.065	0.000	0	13855.	1551.1	8.9	827.	31.9	2270	453	78	-0.112	929
4	0.0756	3.64	0.078	0.056	0.070	0.000	0	10209.	1261.0	8.1	646.	30.5	2916	543	78	-0.102	1223
5	0.0945	3.25	0.093	0.071	0.073	0.000	0	4503.	669.4	6.7	355.	23.3	3322	615	84	-0.055	1445
6	0.1134	2.97	0.115	0.101	0.077	0.000	0	2429.	431.9	5.6	263.	17.3	3634	668	82	-0.019	1679
7	0.1323	2.75	0.148	0.106	0.080	0.000	0	1370.	313.3	4.4	231.	11.8	4081	743	78	0.010	1855
8	0.1512	2.57	0.186	0.149	0.083	0.000	0	768.	211.5	3.6	225.	7.3	4356	793	78	-0.010	1985
9	0.1701	2.42	0.254	0.162	0.086	0.000	0	467.	175.1	2.7	235.	4.6	4544	829	78	0.018	2038
10	0.1890	2.30	0.354	0.232	0.090	0.000	0	317.	161.4	2.0	248.	2.9	4578	872	72	-0.021	1956

Overall: 0.090 0.071 0.090 0.000 0 3708. 683.2 5.4 351. 15.6 31913 5990 756 -0.083 13904  
Rfac Rfull Rcum Ranom Nanom Av\_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS Nbias

Data were good enough to phase data at 2.6 A resolution and model building is in progress.

A complete data set of human Cellular Retinol Binding Protein IV (a new form of CRBP) have been collected. Crystal was very small (about 0.3x0.01x0.01 mm<sup>3</sup>) and twinned, which explains why statistics are not ideal. The structure has been solved by molecular replacement and the R factor is 0.22 (Rfree 0.26).

### CRBP IV

	N	1/d <sup>2</sup>	Dmin(A)	Rfac	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS
1	0.0250	6.32	0.077	0.053	0.077	0.000	0	56622.	7375.0	7.7	3621.	20.9	335	125	0	-0.330	49
2	0.0500	4.47	0.083	0.105	0.082	0.000	0	78847.	11730.2	6.7	5345.	21.5	850	287	0	-0.292	99
3	0.0750	3.65	0.089	0.120	0.086	0.000	0	89909.	12919.5	7.0	6531.	20.5	1211	395	0	-0.230	173
4	0.1000	3.16	0.109	0.109	0.094	0.000	0	57772.	10084.8	5.7	4769.	17.9	1699	535	0	-0.256	298
5	0.1250	2.83	0.132	0.146	0.099	0.000	0	26046.	5452.1	4.8	3028.	14.0	1991	609	0	-0.205	392
6	0.1500	2.58	0.159	0.126	0.104	0.000	0	12856.	3462.2	3.7	2434.	10.4	2227	682	0	-0.241	442
7	0.1750	2.39	0.190	0.148	0.109	0.000	0	8286.	2819.7	2.9	2421.	8.5	2480	778	0	-0.267	507
8	0.2000	2.24	0.220	0.189	0.114	0.000	0	7004.	2896.3	2.4	2564.	7.5	2648	835	1	-0.275	535
9	0.2250	2.11	0.271	0.211	0.118	0.000	0	4749.	2456.2	1.9	2527.	6.1	2796	876	1	-0.197	599
10	0.2500	2.00	0.382	0.321	0.124	0.000	0	3029.	2415.3	1.3	2682.	4.7	2891	932	0	-0.260	596
Overall:		0.124	0.136	0.124	0.000	0	22723.	5925.6	3.8	3180.	11.0	19128	6054	2	-0.246	3690	
		Rfac	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias	

