	Experiment title: Heavy-atom derivatives sf DG741	**Experiment number**: MX-342
Beamline: ID29	**Date of experiment**: from: 17-2-05 to: 18-2-05	**Date of report**: 12-04-05
Shifts: 3	**Local contact(s)**:	*Received at ESRF:*

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Report:

The experiment is aimed at solving the structure of DG741, a protein of the external surface of N. meningitidis. The protein has only one Met, so heavy-atom derivatives were serchead. 4 of them were meausred. The first one is HMPS.

N	1/d^2	Dmin(A)	Rmrg	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias
1	0.0160	7.91	0.049	0.000	0.049	0.039	238	2858.	291.6	9.8	179.	33.8	2072	351	112	0.002	631
2	0.0320	5.59	0.053	0.000	0.051	0.030	490	1691.	141.5	11.9	126.	30.5	4083	600	112	-0.001	1286
3	0.0480	4.56	0.046	0.000	0.049	0.021	643	2781.	210.2	13.2	217.	29.2	5276	754	112	-0.009	1653
4	0.0640	3.95	0.051	0.000	0.049	0.021	780	3117.	248.8	12.5	252.	28.5	6306	887	113	-0.008	1978
5	0.0800	3.54	0.064	0.000	0.053	0.026	888	2377.	221.4	10.7	217.	24.7	7109	996	113	0.013	2248
6	0.0960	3.23	0.086	0.000	0.059	0.035	981	1696.	203.9	8.3	198.	20.1	7838	1082	111	0.012	2585
7	0.1120	2.99	0.117	0.000	0.066	0.048	1088	1155.	187.7	6.1	195.	14.5	8651	1189	109	-0.011	2971
8	0.1280	2.80	0.171	0.000	0.073	0.067	1155	747.	175.7	4.3	188.	10.5	9174	1257	108	-0.017	3086
9	0.1440	2.64	0.245	0.000	0.082	0.098	1246	538.	181.6	3.0	192.	7.7	9806	1342	110	-0.042	3209
10	0.1600	2.50	0.335	0.000	0.093	0.118	1314	410.	186.5	2.2	205.	5.8	10354	1406	103	-0.060	3479
Overall:			0.093	0.000	0.093	0.039	8823	1467.	200.0	7.3	200.	17.5	70669	9864	1103	-0.006	23126

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

N	1/resol^2	Dmin	Nmeas	Nref	Ncent	%poss	C%poss	MIplct	AnoCmpl	AnoFrc	AnoMlt	Rmeas	Rmeas0 (Rsym)	PCV	PCV0	$$	$$
1	0.016	7.91	2087	358	117	99.2	99.2	5.8	99.0	99.0	3.6	0.059	0.067	0.049	0.071	0.089	
2	0.032	5.59	4104	609	118	99.2	99.2	6.7	99.8	99.8	3.7	0.062	0.066	0.053	0.071	0.078	
3	0.048	4.56	5295	766	121	99.4	99.3	6.9	99.5	99.5	3.8	0.054	0.054	0.046	0.061	0.066	
4	0.064	3.95	6326	897	117	99.2	99.3	7.1	99.7	99.9	3.7	0.059	0.059	0.051	0.068	0.072	
5	0.080	3.54	7136	1007	118	99.0	99.2	7.1	99.4	99.7	3.7	0.074	0.074	0.064	0.086	0.091	
6	0.096	3.23	7873	1099	117	99.2	99.2	7.2	99.5	99.6	3.8	0.100	0.099	0.086	0.116	0.122	
7	0.112	2.99	8692	1209	118	98.9	99.1	7.2	99.1	99.6	3.8	0.136	0.136	0.117	0.161	0.171	
8	0.128	2.80	9203	1272	114	98.6	99.0	7.2	98.8	99.4	3.8	0.199	0.197	0.171	0.239	0.248	
9	0.144	2.64	9859	1369	120	99.3	99.1	7.2	99.3	99.8	3.8	0.285	0.283	0.245	0.351	0.365	
10	0.160	2.50	10394	1424	108	98.2	99.0	7.3	98.6	99.7	3.8	0.389	0.382	0.335	0.481	0.493	
Overall			70969	10010	1168	99.0	99.0	7.1	99.2	99.6	3.8	0.108	0.108	0.093	0.127	0.132	

	Nmeas	Nref	Ncent	%poss	C%poss	MIplct	AnoCmpl	AnoFrc	AnoMlt	Rmeas	Rmeas0 (Rsym)	PCV	PCV0

A second heavy-atom derivative was Gd.

N 1/d^2 Dmin(A) Rmrg Rfull Rcum Ranom Nanom Av_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS Nbias
$$
1 0.0160 7.91 0.054 0.054 0.054 0.027 243 2394. 245.3 9.8 188. 35.6 3141 362 117 -0.059 1806
2 0.0320 5.59 0.063 0.064 0.059 0.030 500 1397. 135.4 10.3 116. 33.7 6297 624 124 -0.015 3772
3 0.0480 4.56 0.058 0.052 0.059 0.021 659 2565. 240.3 10.7 221. 34.8 8144 783 124 -0.013 5074
4 0.0640 3.95 0.063 0.056 0.060 0.021 787 2897. 278.6 10.4 277. 31.9 9636 907 120 -0.002 5928
5 0.0800 3.54 0.078 0.057 0.065 0.024 913 2311. 269.8 8.6 260. 26.3 11050 1029 119 -0.007 6867
6 0.0960 3.23 0.100 0.070 0.072 0.031 996 1661. 234.3 7.1 236. 20.8 12101 1120 124 -0.018 7359
7 0.1120 2.99 0.129 0.097 0.078 0.040 1105 1143. 200.7 5.7 214. 16.1 13266 1223 119 -0.015 8253
8 0.1280 2.80 0.182 0.129 0.086 0.057 1197 736. 178.7 4.1 193. 12.0 14315 1311 115 -0.015 8727
9 0.1440 2.64 0.252 0.180 0.096 0.081 1269 535. 181.3 3.0 192. 9.2 15186 1389 122 -0.056 9545
10 0.1600 2.50 0.331 0.231 0.106 0.105 1344 418. 185.8 2.3 202. 7.2 15957 1456 114 -0.061 10008
$$
">For inline graphs use a Java browser</applet>

Overall: 0.106 0.083 0.106 0.035 9013 1386. 214.8 6.5 213. 19.5 109093 10204 1198 -0.018 67339
Rmrg Rfull Rcum Ranom Nanom Av_I SIGMA I/sigma sd Mn(I)/sd Nmeas Nref Ncent FRCBIAS Nbias

N 1/resol^2 Dmin Nmeas Nref Ncent %poss C%poss Mlplct AnoCmpl AnoFrc AnoMlt Rmeas Rmeas0 (Rsym) PCV PCV0 $$
$$
1 0.016 7.91 3148 363 117 99.2 99.2 8.7 99.0 99.0 5.1 0.060 0.063 0.054 0.075 0.085
2 0.032 5.59 6300 627 127 99.9 99.6 10.0 100.0 100.0 5.5 0.069 0.072 0.063 0.082 0.088
3 0.048 4.56 8149 788 129 99.9 99.8 10.3 100.0 100.0 5.5 0.064 0.064 0.058 0.077 0.080
4 0.064 3.95 9643 913 126 99.9 99.8 10.6 100.0 100.0 5.5 0.069 0.069 0.063 0.083 0.086
5 0.080 3.54 11061 1037 124 99.8 99.8 10.7 100.0 100.0 5.5 0.086 0.085 0.078 0.105 0.108
6 0.096 3.23 12108 1126 128 99.8 99.8 10.8 99.8 99.8 5.5 0.110 0.108 0.100 0.134 0.137
7 0.112 2.99 13275 1228 122 99.9 99.8 10.8 99.9 99.9 5.5 0.142 0.141 0.129 0.174 0.180
8 0.128 2.80 14331 1323 122 99.7 99.8 10.8 99.6 99.6 5.5 0.200 0.199 0.182 0.249 0.257
9 0.144 2.64 15195 1395 124 99.5 99.8 10.9 99.7 99.8 5.4 0.278 0.276 0.252 0.354 0.361
10 0.160 2.50 15978 1469 121 99.7 99.7 10.9 99.6 99.6 5.4 0.365 0.362 0.331 0.464 0.478
$$
">For inline graphs use a Java browser</applet>

Overall 109188 10269 1240 99.7 99.7 10.6 99.8 99.8 5.5 0.117 0.116 0.106 0.143 0.146
Nmeas Nref Ncent %poss C%poss Mlplct AnoCmpl AnoFrc AnoMlt Rmeas Rmeas0 (Rsym) PCV PCV0

Analysis of data is inj progress.