

MDO protein G

Regarding the MAD mdog project, four data sets have been collected successfully:

Three data sets were collected at the Se peak, inflexion and remote energy, respectively.

A last data set was measured at the peak energy with a 2 theta angle of 5 degrees for high resolution.

The space group is P212121, with unit cell parameters  
63.86 88.12 215.65 90 90 90

1. data set at the Se peak energy (0.9793); distance 210 mm;  
oscillation 0.7 deg; 257 images

data processed with XDS

data collection statistics:

RESOLUTION	NUMBER OF REFLECTIONS			COMPL	R-FACT	I/SIGI	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	DATA			
10.00	4213	1103	1109	99.5%	4.1%	25.30	1.60
6.00	17688	4527	4575	99.0%	4.8%	22.27	1.57
5.00	16431	4199	4244	98.9%	5.4%	19.92	1.36
4.00	37073	9510	9611	98.9%	5.7%	18.39	1.18
3.00	98282	25399	27060	93.9%	8.1%	12.58	1.11
2.90	15860	4123	4990	82.6%	15.2	8.19	1.07
2.85	8552	2225	2796	79.6%	16.7%	7.61	1.06
2.80	8484	2213	2974	74.4%	18.8%	7.09	1.06
total	206583	53299	57518	92.7%	6.9%	14.50	1.19

2. data set at the Se inflexion energy (0.979494); distance 210 mm,  
oscillation 0.7 deg; 257 images

data processed with XDS

data collection statistics:

RESOLUTION	NUMBER OF REFLECTIONS			COMPL	R-FACT	I/SIGI	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	DATA			
10.00	4258	1112	1112	100.0%	4.0%	25.47	1.24
6.00	17889	4585	4585	100.0%	4.8%	21.76	1.23
5.00	16617	4247	4247	100.0%	5.4%	19.70	1.13
4.00	37569	9637	9638	100.0%	5.8%	17.75	1.05
3.00	104838	27107	27107	100.0%	8.6%	11.55	1.03
2.90	19315	5010	5010	100.0%	17.6%	6.70	1.02
2.85	10790	2799	2799	100.0%	19.9%	6.09	1.01
2.80	11378	2960	2960	100.0%	22.9%	5.46	1.02
total	222654	57457	57617	99.7%	7.3%	13.27	1.06

3. data collected at a Se remote energy (0.973944); distance 210 mm;  
oscillation 0.7 deg; 257 images

data processed with XDS

data collection statistics:

RESOLUTION	NUMBER OF REFLECTIONS			COMPL	R-FACT	I/SIGI	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	DATA			
10.00	4225	1112	1112	100.0%	4.6%	23.44	1.22
6.00	17952	4599	4599	100.0%	5.3%	20.67	1.21
5.00	16619	4253	4253	100.0%	5.9%	18.65	1.12
4.00	37600	9649	9649	100.0%	6.2%	17.11	1.06
3.00	105131	27181	27181	100.0%	8.7%	11.69	1.03
2.90	19218	5004	5004	100.0%	16.1%	7.24	1.02
2.85	10802	2805	2805	100.0%	17.9%	6.71	1.02
2.80	11270	2945	2945	100.0%	20.4%	6.08	1.02
total	222817	57548	57707	99.7%	7.5%	13.14	1.06

4. data collected at the Se peak energy with a 2theta offset to measure higher resolution; 2theta=5deg; distance=210mm  
oscillation=0.7deg; 257 images for a total of 180 deg

data processed with XDS  
data collection statistics:

RESOLUTION	NUMBER OF REFLECTIONS			COMPL	R-FACT	I/SIGI	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	DATA			
10.00	2467	499	666	74.9%	9.3%	13.24	2.21
6.00	16143	2447	2563	95.5%	8.0%	17.69	1.64
5.00	16152	2307	2321	99.4%	7.1%	20.12	1.38
4.00	35985	5120	5169	99.1%	6.3%	23.15	1.20
3.00	84116	14325	14358	99.8%	8.0%	16.07	1.09
2.80	21342	5618	5635	99.7%	8.6%	11.78	1.16
2.50	43711	12054	12232	98.5%	9.4%	10.50	1.16
2.49	1678	476	507	93.9%	10.7%	9.20	1.13
total	221594	42846	43565	98.3%	7.4%	14.99	1.18

The structure has been solved by MAD with the three wavelengths using CNS.

In parallel, the structure has also been solved using only the Se peak data. In this case, the Se substructure has been resolved with shelxd at 3.1 A resolution (CC=0.43).

The crystal contains two molecules/au. Each molecule contains 498 residues, with ten methionines.

The shelxd solution has been confirmed and the NCS operation determined with PROFESS from CCP4

The Se substructure has been refined and the SAD structure phased with SHARP, density modification including averaging with solomon and DM.

The chain has been autotraced partially with ARP/WARP.

Reconstruction and final refinements are in progress.

We have also collected a high resolution data set for another project FHA30, for which the structure has been determined in the lab by MIRAS to 2.2 A resolution.

Project Fha30; high resolution data; wave=(0.979337A); oscillation 1 deg;

360 images; distance 125mm

cell:108.983 43.043 53.796 90.000 104.074 90.000  
symmetry c2

data processed with XDS:

RESOLUTION	NUMBER OF REFLECTIONS			COMPL	R-FACT	I/SIGI	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	DATA			
10.00	727	125	149	83.9%	2.8%	53.60	0.99
6.00	4070	504	508	99.2%	5.3%	45.74	0.98
5.00	4193	460	460	100.0%	6.4%	37.00	0.98
4.00	9384	1034	1040	99.4%	6.0%	31.11	0.98
3.00	28715	2838	2846	99.7%	8.2%	23.46	0.97
2.40	48737	4674	4682	99.8%	10.2%	27.67	0.97
1.90	64417	9602	9651	99.5%	8.9%	24.09	0.99
1.72	29839	6534	6600	99.0%	13.9%	9.56	0.95
total	190082	25771	25936	99.4%	8.3%	22.07	0.97

Final refinements are in progress.

No problem encountered on the beam line. Very good help from the beam line staff.