Crystallization of Mitochondrial Respiratory Complex II from Chicken Heart: a Membrane Protein Complex Diffracting to 2.0 Å.

Li-shar Huang, Toni M. Borders, John T. Shen, Chung-Jen Wang and Edward Berry

MS TS4050 Supplemental Material: analysis of I/sig(I), Chi^2, and R-merge vs resolution. SCALEPACK and TRUNCATE log files for the dataset described in Table 1.

1. Tail of Scalepack logfile with statistics by shell:

film	nrefl	nrefl >1	I/sigI	Chi^2	R-sym
717	530	525	21.3	1.313	0.123
718	516	513	24.4	1.331	0.122
719	372	370	21.3	1.493	0.134
720	0	0	0.0	0.000	0.000
All films	**342303**	**334891**	**22.7**	**1.109**	**0.116**

Summary of observation redundancies by shells:

Shell Lower limit	Upper limit	No. of reflections with given No. of observations 0	1	2	3	4	5-6	7-8	9-12	13-19	>19	total
99.00	4.71	41	28	162	499	1260	1864	5699	0	0	0	9512
4.71	3.74	3	10	149	452	928	2932	4712	0	0	0	9183
3.74	3.27	14	149	552	1128	1546	3211	2499	0	0	0	9085
3.27	2.97	173	674	1188	1518	1298	2128	2053	0	0	0	8859
2.97	2.76	485	798	1265	1313	1072	2061	2013	0	0	0	8522
2.76	2.59	652	805	1365	1150	1152	2299	1584	0	0	0	8355
2.59	2.46	1102	1059	2026	1524	1831	1252	144	0	0	0	7836
2.46	2.36	2010	1170	2693	1401	1216	383	50	0	0	0	6913
2.36	2.27	2997	1375	2867	1057	498	171	18	0	0	0	5986
2.27	2.19	4684	1344	2225	455	154	60	7	0	0	0	4245
All hkl		12161	7412	14492	10497	10955	16361	18779	0	0	0	78496

Average Redundancy Per Shell

Shell Lower limit	Upper limit	
99.00	4.71	6.4
4.71	3.74	6.2
3.74	3.27	5.2
3.27	2.97	4.5
2.97	2.76	4.4
2.76	2.59	4.3
2.59	2.46	3.2
2.46	2.36	2.6
2.36	2.27	2.2
2.27	2.19	1.9
All hkl		4.4

Summary of observation redundancies:

Shell Lower limit	Upper limit	% of reflections with given No. of observations 0	1	2	3	4	5-6	7-8	9-12	13-19	>19	total
99.00	4.71	0.4	0.3	1.7	5.2	13.2	19.5	59.7	0.0	0.0	0.0	99.6
4.71	3.74	0.0	0.1	1.6	4.9	10.1	31.9	51.3	0.0	0.0	0.0	100.0
3.74	3.27	0.2	1.6	6.1	12.4	17.0	35.3	27.5	0.0	0.0	0.0	99.8
3.27	2.97	1.9	7.5	13.2	16.8	14.4	23.6	22.7	0.0	0.0	0.0	98.1

2.97	2.76	5.4	8.9	14.0	14.6	11.9	22.9	22.3	0.0	0.0	0.0	94.6
2.76	2.59	7.2	8.9	15.2	12.8	12.8	25.5	17.6	0.0	0.0	0.0	92.8
2.59	2.46	12.3	11.8	22.7	17.1	20.5	14.0	1.6	0.0	0.0	0.0	87.7
2.46	2.36	22.5	13.1	30.2	15.7	13.6	4.3	0.6	0.0	0.0	0.0	77.5
2.36	2.27	33.4	15.3	31.9	11.8	5.5	1.9	0.2	0.0	0.0	0.0	66.6
2.27	2.19	52.5	15.1	24.9	5.1	1.7	0.7	0.1	0.0	0.0	0.0	47.5
All hkl		13.4	8.2	16.0	11.6	12.1	18.0	20.7	0.0	0.0	0.0	86.6

Shell I/Sigma in resolution shells:

Lower limit	Upper limit	No. of reflections with I / Sigma less than 0	1	2	3	5	10	20	>20	total
99.00	4.71	2	6	12	21	51	856	9512	0	9512
4.71	3.74	1	6	12	19	48	838	9183	0	9183
3.74	3.27	6	9	27	53	196	2457	9085	0	9085
3.27	2.97	31	79	169	301	866	4525	8859	0	8859
2.97	2.76	58	158	358	639	1584	5077	8522	0	8522
2.76	2.59	96	297	620	1076	2337	5824	8355	0	8355
2.59	2.46	190	527	1138	1841	3537	7038	7836	0	7836
2.46	2.36	251	806	1635	2542	4334	6767	6913	0	6913
2.36	2.27	410	1060	1982	2936	4487	5971	5986	0	5986
2.27	2.19	361	1026	1911	2680	3722	4244	4245	0	4245
All hkl		1406	3974	7864	12108	21162	43597	78496	0	78496

Shell I/Sigma in resolution shells:

Lower limit	Upper limit	% of of reflections with I / Sigma less than 0	1	2	3	5	10	20	>20	total
99.00	4.71	0.0	0.1	0.1	0.2	0.5	9.0	99.6	0.0	99.6
4.71	3.74	0.0	0.1	0.1	0.2	0.5	9.1	100.0	0.0	100.0
3.74	3.27	0.1	0.1	0.3	0.6	2.2	27.0	99.8	0.0	99.8
3.27	2.97	0.3	0.9	1.9	3.3	9.6	50.1	98.1	0.0	98.1
2.97	2.76	0.6	1.8	4.0	7.1	17.6	56.4	94.6	0.0	94.6
2.76	2.59	1.1	3.3	6.9	11.9	25.9	64.7	92.8	0.0	92.8
2.59	2.46	2.1	5.9	12.7	20.6	39.6	78.7	87.7	0.0	87.7
2.46	2.36	2.8	9.0	18.3	28.5	48.6	75.8	77.5	0.0	77.5
2.36	2.27	4.6	11.8	22.1	32.7	49.9	66.5	66.6	0.0	66.6
2.27	2.19	4.0	11.5	21.4	30.0	41.7	47.5	47.5	0.0	47.5
All hkl		1.6	4.4	8.7	13.4	23.3	48.1	86.6	0.0	86.6

Summary of reflections intensities and R-factors by shells

R linear = SUM (ABS(I - <I>)) / SUM (I)

R square = SUM ((I - <I>) ** 2) / SUM (I ** 2)

Chi**2 = SUM ((I - <I>) ** 2) / (Error ** 2 * N / (N-1)))

In all sums single measurements are excluded

Shell limit	Lower Angstrom	Upper	Average I	Average error	Average stat.	Norm. Chi**2	Linear R-fac	Square R-fac
99.00	4.71		21104.0	1593.1	159.4	0.828	0.096	0.107
4.71	3.74		17160.1	1283.2	154.1	1.090	0.120	0.140
3.74	3.27		8959.9	739.2	137.9	1.241	0.130	0.153
3.27	2.97		4081.3	377.5	121.9	1.310	0.141	0.163
2.97	2.76		2431.3	240.7	102.5	1.287	0.152	0.174
2.76	2.59		1628.0	179.4	93.9	1.214	0.162	0.175
2.59	2.46		1162.2	177.3	116.0	1.125	0.170	0.175
2.46	2.36		831.6	170.3	131.9	1.036	0.197	0.184
2.36	2.27		665.2	173.8	147.0	0.995	0.220	0.198
2.27	2.19		491.7	175.8	160.7	0.974	0.270	0.242
All reflections			6766.3	572.0	131.3	1.117	0.116	0.125

2. Tail of "truncate" logfile with statistics by shell:

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 $TABLE: Amplitude analysis against resolution:
 $GRAPHS:Mn(F) v. resolution:N:2,9::Mn(F/sd) v. resolution:N:2,12:
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Range	1/resol^2	Dmax	Nref	Mn(I)	Mn(sd)	Mn(I)/Mn(sd)	Mn(I/sd)	Mn(F)	Mn(sd)	Mn(F)/Mn(sd)	Mn(F/sd)
1	0.0041	15.55	284	51918.83	3950.59	13.14	15.48	948.59	36.00	26.35	30.73
2	0.0076	11.47	420	38461.42	2363.47	16.27	17.35	804.53	24.95	32.25	34.53
3	0.0111	9.51	517	47431.80	2897.36	16.37	18.00	894.72	27.08	33.04	35.83
4	0.0145	8.30	595	37425.66	2246.58	16.66	18.18	796.09	23.86	33.36	36.19
5	0.0180	7.45	662	26134.72	1569.56	16.65	18.46	666.27	19.54	34.09	36.78
6	0.0215	6.83	712	16438.90	992.31	16.57	18.11	536.31	16.07	33.36	36.07
7	0.0249	6.33	772	12173.41	716.75	16.98	18.30	462.44	13.55	34.12	36.47
8	0.0284	5.93	838	12597.69	732.99	17.19	18.36	467.67	13.65	34.27	36.57
9	0.0319	5.60	878	12271.25	701.42	17.49	18.47	464.80	13.38	34.74	36.80
10	0.0353	5.32	913	14167.15	807.14	17.55	18.46	497.39	14.25	34.91	36.78
11	0.0388	5.08	972	15078.66	856.82	17.60	18.65	512.87	14.55	35.24	37.15
12	0.0423	4.86	1009	18232.38	1055.07	17.28	18.65	555.94	15.86	35.04	37.16
13	0.0457	4.68	1020	18706.11	1043.78	17.92	18.72	572.38	16.12	35.52	37.30
14	0.0492	4.51	1112	18838.53	1056.99	17.82	18.66	575.20	16.25	35.39	37.18
15	0.0527	4.36	1094	19904.69	1138.06	17.49	18.52	585.91	16.65	35.19	36.90
16	0.0561	4.22	1156	18998.47	1064.88	17.84	18.60	565.75	15.91	35.57	37.08
17	0.0596	4.10	1190	17430.20	971.68	17.94	18.26	546.67	15.56	35.13	36.39
18	0.0631	3.98	1227	16095.69	924.47	17.41	18.24	534.50	15.38	34.76	36.35
19	0.0665	3.88	1243	15978.24	938.94	17.02	17.87	523.18	15.43	33.92	35.61
20	0.0700	3.78	1286	13515.05	786.54	17.18	17.79	489.95	14.45	33.91	35.45
21	0.0734	3.69	1301	11800.51	701.19	16.83	17.33	453.23	13.70	33.08	34.52
22	0.0769	3.61	1381	11371.32	685.50	16.59	16.95	444.12	13.71	32.39	33.75
23	0.0804	3.53	1331	10031.73	609.57	16.46	16.55	419.80	13.23	31.74	32.96
24	0.0838	3.45	1431	8671.94	539.67	16.07	15.93	388.09	12.78	30.36	31.72
25	0.0873	3.38	1416	7664.27	498.21	15.38	15.52	366.11	12.51	29.26	30.89
26	0.0908	3.32	1430	6827.86	448.97	15.21	15.07	342.62	12.09	28.35	29.99
27	0.0942	3.26	1502	6000.73	401.53	14.94	14.55	324.12	11.82	27.43	28.95
28	0.0977	3.20	1488	5205.53	348.68	14.93	14.15	299.10	11.29	26.49	28.15
29	0.1012	3.14	1514	4280.69	302.92	14.13	13.68	272.52	10.88	25.05	27.20
30	0.1046	3.09	1567	3745.18	263.13	14.23	13.27	255.26	10.37	24.61	26.40
31	0.1081	3.04	1523	3582.65	254.46	14.08	13.23	249.66	10.24	24.39	26.31
32	0.1116	2.99	1618	3291.83	242.30	13.59	12.60	235.80	10.36	22.76	25.06
33	0.1150	2.95	1580	2802.47	212.40	13.19	12.53	220.26	9.78	22.53	24.91
34	0.1185	2.90	1595	2542.38	190.92	13.32	12.00	206.73	9.54	21.66	23.86
35	0.1220	2.86	1637	2343.30	182.46	12.84	11.95	202.03	9.54	21.17	23.74
36	0.1254	2.82	1646	2338.62	178.35	13.11	12.00	200.36	9.41	21.29	23.85
37	0.1289	2.79	1651	2032.77	157.82	12.88	11.60	186.72	9.12	20.47	23.07
38	0.1324	2.75	1678	1937.77	154.62	12.53	11.20	180.74	9.31	19.42	22.27
39	0.1358	2.71	1705	1762.62	141.97	12.42	10.88	171.81	9.10	18.88	21.64
40	0.1393	2.68	1675	1622.65	133.17	12.19	10.76	165.29	8.83	18.71	21.41
41	0.1428	2.65	1754	1430.43	122.24	11.70	10.24	156.13	8.86	17.61	20.35
42	0.1462	2.62	1722	1388.74	125.15	11.10	9.89	153.09	9.11	16.80	19.67
43	0.1497	2.58	1762	1281.80	126.94	10.10	8.90	147.07	9.59	15.33	17.70
44	0.1532	2.56	1736	1143.13	128.46	8.90	7.98	138.73	10.37	13.37	15.81
45	0.1566	2.53	1747	1178.07	142.68	8.26	7.58	140.26	11.08	12.66	15.05
46	0.1601	2.50	1673	980.47	133.54	7.34	6.81	128.59	11.52	11.17	13.52
47	0.1636	2.47	1665	963.27	138.66	6.95	6.49	127.50	11.97	10.66	12.86
48	0.1670	2.45	1667	867.35	134.00	6.47	6.00	120.73	12.38	9.75	11.87
49	0.1705	2.42	1630	794.25	134.17	5.92	5.51	115.78	12.82	9.03	10.90

50	0.1740	2.40	1532	760.84	135.77	5.60	5.22	112.89	13.19	8.56	10.38
51	0.1774	2.37	1583	710.50	136.58	5.20	4.87	109.17	13.83	7.89	9.63
52	0.1809	2.35	1505	683.42	138.02	4.95	4.65	107.15	14.05	7.62	9.24
53	0.1843	2.33	1450	591.10	131.76	4.49	4.22	100.47	14.34	7.01	8.40
54	0.1878	2.31	1458	624.10	141.38	4.41	4.13	102.29	15.05	6.80	8.22
55	0.1913	2.29	1405	579.92	142.62	4.07	3.77	98.34	15.56	6.32	7.55
56	0.1947	2.27	1389	555.86	145.16	3.83	3.63	96.55	15.93	6.06	7.30
57	0.1982	2.25	1332	506.13	142.96	3.54	3.36	92.23	16.29	5.66	6.73
58	0.2017	2.23	1328	430.67	142.89	3.01	2.89	84.88	17.07	4.97	5.88
59	0.2051	2.21	1273	398.19	143.85	2.77	2.72	82.63	17.44	4.74	5.49
60	0.2086	2.19	984	433.81	162.36	2.67	2.55	85.04	18.83	4.51	5.18
TOTALS			79164	6527.89	432.70	15.09	11.59	279.07	12.98	21.50	23.07

Minimum F = 12.799
with SD = 6.476
Maximum F = 3667.282
with SD = 254.218

ANALYSIS OF THE ANISOTROPY OF THE DATA ACCORDING TO THE FALLOFF PROCEDURE.

Direction 1 is perpendicular to b* and Direction 3
Direction 2 is along b*
Direction 3 is perpendicular to a* and b*

$TABLE: Anisotropy analysis (FALLOFF). truncate :
$GRAPHS:Mn(F) v. resolution:A:1,2,3,4,5:: Mn(F/sd) v. resolution:A:1,6,7,8,9:: No. reflections v. resolution:A:1,10,11,12,13:
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1/resol^2	Mn(F(d1))	Mn(F(d2))	Mn(F(d3))	Mn(F(ov))	Mn(F/sd(d1))	Mn(F/sd(d2))	Mn(F/sd(d3))	Mn(F/sd(ov))	N(d1)	N(d2)	N(d3)	N(ov)
0.00348	1004.71	952.07	863.80	1008.23	24.48	22.80	21.53	26.12	232	208	280	1696
0.00695	766.91	693.13	749.90	774.94	30.71	27.17	24.92	30.50	464	472	512	3176
0.01043	790.61	873.73	937.93	851.34	30.02	29.63	27.08	31.88	544	592	632	4080
0.01391	861.17	862.96	843.41	808.90	32.30	31.06	27.96	33.21	672	592	696	4592
0.01738	689.47	696.40	717.50	698.78	33.85	30.43	28.63	33.48	768	768	800	5296
0.02086	534.55	546.05	516.02	545.81	32.49	31.21	29.07	33.43	704	808	816	5632
0.02434	466.19	430.73	485.87	469.79	34.40	31.45	28.57	33.66	784	848	936	6056
0.02781	403.42	474.80	515.71	467.52	33.66	32.03	29.64	33.93	1000	928	952	6688
0.03129	441.33	441.95	499.61	463.29	33.25	32.58	30.30	34.36	936	976	1032	6992
0.03477	442.74	443.00	515.42	482.95	34.05	32.38	30.98	34.58	928	976	1048	7296
0.03824	520.91	422.76	588.85	516.10	35.23	32.32	30.49	34.69	1144	1144	1144	7760
0.04172	454.10	458.96	732.47	546.27	33.52	32.54	31.14	34.63	1072	1136	1128	8016
0.04520	533.57	459.90	698.92	569.39	36.57	34.18	31.77	35.58	1112	992	1200	8176
0.04868	549.83	483.48	676.08	572.86	34.13	32.22	31.70	34.94	1192	1344	1232	8728
0.05215	534.98	448.64	752.24	578.55	36.49	32.24	31.28	35.01	1152	1208	1296	8808
0.05563	485.74	449.63	812.17	576.13	33.64	34.16	31.61	34.91	1336	1192	1288	9240
0.05911	516.72	417.10	706.01	540.21	34.82	32.02	32.23	34.47	1128	1424	1456	9632
0.06258	546.50	452.95	713.47	533.66	34.89	32.79	31.93	34.50	1584	1264	1376	9824
0.06606	482.92	424.17	710.03	529.03	35.06	32.52	32.46	34.12	1136	1392	1408	9824
0.06954	507.89	408.93	576.48	496.93	33.37	31.01	31.80	33.50	1680	1448	1472	10408
0.07301	406.97	353.56	606.63	453.25	33.48	32.04	32.01	33.07	1136	1408	1488	10392
0.07649	400.41	325.13	622.53	449.63	31.49	29.72	32.00	32.33	1680	1528	1504	10936
0.07997	409.69	316.42	555.44	424.37	32.45	29.69	32.27	31.77	1424	1408	1552	10712
0.08344	347.51	293.08	541.59	392.42	27.41	27.83	32.33	30.19	1496	1680	1552	11480
0.08692	337.36	298.41	466.13	367.08	29.10	27.59	30.93	29.76	1688	1400	1656	11416
0.09040	358.62	255.59	468.62	348.56	27.70	24.24	31.21	28.87	1328	1768	1648	11336
0.09387	310.51	257.27	430.92	327.98	25.03	25.58	30.32	27.72	1728	1408	1728	12184
0.09735	265.29	223.31	402.72	294.73	23.96	21.76	30.99	27.11	1672	1760	1672	11848
0.10083	248.81	204.91	368.19	274.96	22.17	20.78	29.26	26.03	1624	1600	1736	12160
0.10430	246.56	190.21	349.16	256.55	22.00	19.61	29.42	25.45	1680	1648	1768	12544
0.10778	248.04	188.39	338.29	253.47	22.77	18.97	29.57	25.68	1664	1816	1776	12224
0.11126	226.66	163.98	336.34	234.19	18.53	18.20	28.59	23.78	1736	1544	1864	12968

0.11473	214.40	170.85	299.00	224.50	20.00	18.30	28.71	24.17	1584	1704	1784	12520
0.11821	191.25	159.59	296.22	208.51	19.09	17.67	27.93	23.26	1720	1656	1912	13032
0.12169	188.52	158.93	283.85	201.74	17.87	16.80	28.51	22.87	1736	1680	1800	12976
0.12517	181.09	152.02	281.71	200.37	17.11	17.11	28.19	23.01	1616	1688	2016	13240
0.12864	189.37	131.03	251.93	188.39	18.38	14.96	27.00	22.35	1672	1672	1880	13144
0.13212	176.21	133.08	254.67	181.70	16.76	14.96	27.28	21.75	1896	1664	2016	13528
0.13560	159.74	125.23	254.43	173.12	15.96	14.05	26.13	20.89	1560	1776	1960	13656
0.13907	169.79	120.70	241.81	165.89	18.04	13.96	25.99	20.80	1624	1560	1992	13560
0.14255	158.01	105.58	224.81	156.82	16.86	11.83	25.37	19.77	1896	1688	2072	13944
0.14603	151.36	108.11	237.66	156.55	16.06	12.53	25.02	19.36	1704	1840	2008	13880
0.14950	150.99	106.72	217.45	148.81	16.43	12.34	20.11	17.32	1544	1720	2168	14096
0.15298	135.92	99.84	196.17	140.38	14.78	12.07	16.36	15.53	1816	1688	1976	13896
0.15646	139.03	97.57	198.85	140.10	14.99	10.82	14.60	14.74	2136	1712	2048	14136
0.15993	124.45	97.97	172.28	128.84	13.21	10.50	12.08	13.23	1560	1624	1904	13376
0.16341	112.69	98.81	170.63	128.89	11.68	11.15	10.86	12.72	1640	1552	1752	13368
0.16689	118.58	87.99	161.40	122.08	12.02	9.57	10.19	11.66	2064	1600	1752	13312
0.17036	116.72	82.68	157.33	115.43	11.76	8.89	9.78	10.68	2024	1560	1624	13104
0.17384	110.18	72.10	152.72	112.52	11.22	7.10	9.16	10.22	1520	1288	1424	12384
0.17732	105.88	79.02	151.77	108.70	9.90	7.70	8.86	9.45	1896	1512	1376	12744
0.18079	102.00	69.75	136.65	107.03	9.68	6.82	7.86	9.07	1896	1376	1264	12112
0.18427	101.08	76.50	133.70	100.47	9.42	7.17	7.72	8.32	1864	1136	1016	11608
0.18775	110.11	75.63	134.88	102.24	9.17	6.95	7.48	8.08	1672	1296	1008	11728
0.19122	104.88	66.78	138.04	98.20	8.33	6.33	7.79	7.44	1832	1136	848	11264
0.19470	96.56	73.40	131.71	95.96	7.69	6.81	7.20	7.18	1784	1024	760	11152
0.19818	103.37	65.57	126.09	91.55	8.30	5.63	7.01	6.60	1768	1072	680	10672
0.20166	84.82	60.86	113.92	84.42	6.04	5.03	5.78	5.78	1680	968	624	10624
0.20513	83.73	64.23	96.26	81.94	5.65	5.20	4.90	5.40	1680	944	472	10240
0.20861	86.37	58.89	95.15	84.34	5.76	4.15	4.65	5.09	1208	632	352	7888

Average F (d1 d2 d3) + overall average: 272.92 247.14 396.87 286.25

WARNING: ***Beware-serious ANISOTROPY; data analyses may be invalid *

number A-AX reflections less than 30.0 degrees from dir1 87016
number B-AX reflections less than 30.0 degrees from dir2 79448
number C-AX reflections less than 30.0 degrees from dir3 83136
number overall reflections 633304