

List of observed and calculated structure factors (to be deposited)

<u>_refln_index_h</u>						
<u>_refln_index_k</u>						
<u>_refln_index_l</u>						
<u>_refln_F_squared_calc</u>						
<u>_refln_F_squared_meas</u>						
<u>_refln_F_squared_sigma</u>						
<u>_refln_observed_status</u>						
0	1	0	1963.26	2002.78	41.18	o
-1	2	0	13581.21	15202.77	275.19	o
0	2	0	14.02	28.90	7.88	o
-1	3	0	1180.41	1300.56	25.51	o
0	3	0	8333.62	8777.28	195.61	o
-2	4	0	10778.05	11345.43	221.51	o
-1	4	0	888.16	938.09	30.76	o
0	4	0	91.59	88.10	21.80	o
-2	5	0	599.70	637.11	22.63	o
-1	5	0	3981.19	4003.78	76.98	o
0	5	0	441.76	453.07	48.56	o
-3	6	0	2832.44	2895.69	76.12	o
-2	6	0	91.64	95.14	22.01	o
-1	6	0	411.36	475.49	28.10	o
0	6	0	2793.68	2736.42	115.66	o
-3	7	0	295.88	315.91	29.75	o
-2	7	0	1743.01	1755.96	55.17	o
0	0	1	749.90	655.21	23.78	o
0	1	1	25.69	19.38	5.28	o
-1	2	1	1615.17	1608.03	23.70	o
0	2	1	361.98	371.76	10.75	o
-1	3	1	17.86	20.18	5.16	o
0	3	1	961.14	975.88	31.61	o
-2	4	1	419.62	497.19	24.04	o
-1	4	1	11.20	26.67	8.55	o
0	4	1	95.79	105.58	14.28	o
-2	5	1	11.25	28.33	10.95	o
-1	5	1	489.62	632.21	19.76	o
0	5	1	9.80	15.30	23.59	o
-3	6	1	373.15	485.47	28.61	o
-2	6	1	45.66	53.80	14.64	o
-1	6	1	4.93	20.64	17.48	o
0	6	1	144.87	187.92	28.93	o
-3	7	1	5.66	81.02	20.89	o
-2	7	1	198.47	303.88	25.71	o
0	0	2	9788.41	9752.24	301.72	o
0	1	2	6280.22	5881.73	89.65	o
-1	2	2	2772.64	2546.56	36.83	o
0	2	2	1478.00	1320.33	23.14	o
-1	3	2	3037.58	2978.01	29.95	o
0	3	2	2208.45	2159.62	33.57	o
-2	4	2	3381.44	3328.33	49.37	o
-1	4	2	1923.07	1870.01	23.67	o
0	4	2	741.95	706.57	21.69	o
-2	5	2	1239.08	1216.13	20.48	o
-1	5	2	1272.95	1230.15	24.20	o
0	5	2	855.56	814.03	33.91	o
-3	6	2	958.01	944.26	29.46	o
-2	6	2	393.33	452.39	17.85	o
-1	6	2	678.70	663.79	24.16	o
0	6	2	1081.32	963.07	43.87	o
-3	7	2	475.87	517.42	22.33	o

-2	7	2	662.60	677.85	24.72	o
0	0	3	1932.17	1959.13	120.14	o
0	1	3	1143.82	1055.38	20.98	o
-1	2	3	5289.30	4991.97	67.41	o
0	2	3	3547.12	3434.50	47.01	o
-1	3	3	840.75	785.14	14.07	o
0	3	3	3192.32	3004.00	43.08	o
-2	4	3	1223.52	1202.87	26.17	o
-1	4	3	605.75	605.42	14.50	o
0	4	3	1391.64	1344.01	30.07	o
-2	5	3	498.66	503.20	14.68	o
-1	5	3	1623.37	1556.67	26.30	o
0	5	3	392.28	333.21	23.11	o
-3	6	3	1258.26	1267.70	35.34	o
-2	6	3	727.99	696.66	21.97	o
-1	6	3	255.65	214.47	19.41	o
0	6	3	439.03	469.28	38.60	o
-3	7	3	220.25	197.82	21.43	o
-2	7	3	681.06	642.78	26.84	o
0	0	4	3052.92	3460.57	192.93	o
0	1	4	0.52	-1.67	10.48	o
-1	2	4	2085.26	1990.96	33.44	o
0	2	4	0.45	10.74	9.33	o
-1	3	4	4.29	9.57	8.72	o
0	3	4	1296.14	1294.08	28.59	o
-2	4	4	1108.20	1130.19	26.82	o
-1	4	4	7.84	1.84	10.79	o
0	4	4	5.26	-13.66	15.79	o
-2	5	4	8.99	3.87	12.88	o
-1	5	4	616.64	648.41	18.63	o
0	5	4	9.35	-20.30	20.30	o
-3	6	4	445.58	480.04	31.54	o
-2	6	4	7.09	2.43	16.16	o
-1	6	4	9.74	-18.97	18.97	o
0	6	4	299.55	347.76	42.73	o
-3	7	4	9.20	-17.25	22.62	o
0	0	5	3821.47	4646.20	255.02	o
0	1	5	837.68	780.97	25.34	o
-1	2	5	6438.16	6128.07	88.07	o
0	2	5	2204.60	2101.03	37.60	o
-1	3	5	596.24	589.36	14.86	o
0	3	5	4353.02	4352.23	69.52	o
-2	4	5	2275.26	2217.14	43.02	o
-1	4	5	417.39	440.86	15.04	o
0	4	5	951.08	973.87	29.12	o
-2	5	5	341.20	353.72	15.83	o
-1	5	5	2374.17	2282.47	35.56	o
0	5	5	271.13	267.51	26.17	o
-3	6	5	1851.01	1790.76	50.05	o
-2	6	5	521.33	540.63	21.74	o
-1	6	5	178.33	170.79	20.16	o
0	0	6	1278.93	1349.70	110.41	o
0	1	6	0.54	-17.83	17.83	o
-1	2	6	346.70	316.41	19.27	o
0	2	6	137.27	137.49	19.39	o
-1	3	6	0.02	12.26	13.29	o
0	3	6	240.50	229.37	22.00	o
-2	4	6	474.98	438.08	21.52	o
-1	4	6	0.61	-15.43	15.43	o
0	4	6	39.10	28.48	21.65	o
-2	5	6	0.33	7.48	17.36	o
-1	5	6	111.85	71.64	17.17	o
0	5	6	0.37	-27.36	29.02	o

-3	6	6	74.22	57.60	33.42	o
-2	6	6	15.46	-19.90	19.90	o
-1	6	6	2.29	-21.53	21.64	o
0	0	7	1917.14	2197.94	148.67	o
0	1	7	602.19	644.44	27.04	o
-1	2	7	2219.90	2281.84	54.27	o
0	2	7	850.48	877.16	32.78	o
-1	3	7	449.98	501.06	20.34	o
0	3	7	1569.82	1622.15	50.33	o
-2	4	7	1034.62	1081.49	39.08	o
-1	4	7	333.84	311.33	19.66	o
0	4	7	454.59	496.68	32.98	o
-2	5	7	264.53	194.57	21.57	o
-1	5	7	888.67	905.28	29.13	o
0	5	7	208.63	180.79	32.01	o
-3	6	7	698.86	683.12	43.97	o
-2	6	7	268.61	215.11	25.35	o
0	0	8	1432.44	1726.48	135.54	o
0	1	8	663.87	694.50	35.16	o
-1	2	8	537.90	535.90	31.38	o
0	2	8	154.06	166.98	27.39	o
-1	3	8	455.20	434.16	21.48	o
0	3	8	436.99	444.87	30.37	o
-2	4	8	774.94	822.93	43.75	o
-1	4	8	336.02	320.25	22.83	o
0	4	8	84.38	89.37	33.50	o
-2	5	8	230.70	217.81	25.93	o
-1	5	8	266.57	246.89	24.91	o
0	5	8	166.78	139.37	37.22	o
0	0	9	453.33	566.31	88.68	o
0	1	9	86.18	58.85	32.51	o
-1	2	9	295.10	346.87	34.21	o
0	2	9	36.71	-22.16	29.57	o
-1	3	9	61.74	18.54	22.73	o
0	3	9	228.18	168.17	34.70	o
-2	4	9	257.91	176.32	37.45	o
-1	4	9	46.74	-11.81	23.66	o
0	4	9	20.68	-31.85	37.95	o
-2	5	9	34.13	4.37	27.88	o
-1	5	9	137.45	82.93	27.59	o
0	0	10	1556.03	2173.13	157.42	o
0	1	10	189.09	204.32	37.33	o
-1	2	10	948.22	1236.48	55.01	o
0	2	10	56.44	49.61	40.77	o
-1	3	10	148.91	107.52	27.23	o
0	3	10	722.48	714.59	44.65	o
-2	4	10	867.93	874.50	64.97	o
-1	4	10	122.78	104.52	36.50	o
0	4	10	39.84	15.55	41.91	o
0	0	11	2.48	31.29	87.55	o
0	1	11	0.01	-43.41	43.41	o
-1	2	11	13.64	-6.53	41.43	o
0	2	11	22.73	-43.75	43.75	o
-1	3	11	0.02	-30.13	30.13	o
0	3	11	9.91	-25.77	42.75	o
0	0	12	309.12	78.63	118.84	o
0	1	12	116.23	77.14	69.65	o
-1	2	12	254.36	195.25	51.64	o
0	2	12	88.95	-26.31	59.81	o