Table 8. Observed (FO) and calculated (FC) structure factors for sample 1. Tas27-2Ba.

H	K	L	/FO/	/FC/
3	1	-16	9.1	-9.9
1	3	-16	11.3	11.6
2	6	-15	13.3	-13.5
0	2	-15	11.5	12.5
1	1	-15	10.5	-11.0
-1	1	-15	9.9	-9.2
0	0	-15	16.1	-17.4
2	0	-15	10.1	-10.1
4	0	-14	36.0	38.1
2	0	-14	28.8	30.0
4	2	-14	8.6	-8.9
-1	3	-14	9.7	9.7
3	3	-14	16.9	-16.5
4	6	-14	22.1	22.9
2	6	-14	23.3	23.5
1	9	-13	20.8	-20.8
-1	7	-13	8.7	8.0
0	6	-13	13.5	14.8
2	6	-13	9.9	9.6
4	6	-13	22.8	-21.9
5	5	-13	9.8	-9.1
4	4	-13	13.5	13.4
5	3	-13	11.8	13.3
3	3	-13	11.4	-11.1
1	3	-13	42.5	-42.7
-1	3	-13	26.1	-27.2
2	2	-13	10.6	10.2
6	2	-13	8.6	9.2
0	0	-13	21.1	22.9
4	0	-13	20.9	-19.8
6	0	-13	22.5	-23.3
5	1	-13	8.9	-9.2
1	1	-12	10.4	-10.4
3	1	-12	11.3	-11.6
6	0	-12	21.9	22.9
2	0	-12	16.4	-16.1
0	0	-12	28.8	27.8
4	2	-12	16.1	16.2
2	2	-12	20.1	20.4
1	3	-12	35.5	35.3
3	3	-12	39.2	37.9
5	3	-12	13.7	14.3
4	4	-12	13.6	13.4
2	4	-12	13.8	12.7
0	4	-12	16.2	15.9
1	5	-12	9.1	-9.2
0	6	-12	9.6	9.9
3	7	-12	11.5	-11.5
4	8	-12	8.4	8.2
2	8	-12	9.2	9.4

H	K	L	/FO/	/FC/
1	9	-12	20.3	20.0
3	9	-12	26.9	26.9
0	10	-11	8.8	8.7
3	9	-11	12.9	-11.7
-1	9	-11	10.9	10.8
0	8	-11	12.9	13.9
2	8	-11	11.1	10.6
3	7	-11	9.8	-8.2
0	6	-11	35.2	-34.8
2	6	-11	13.0	-11.8
1	5	-11	16.0	-16.3
-1	5	-11	9.0	-9.4
0	4	-11	23.5	24.0
2	4	-11	16.8	17.5
7	3	-11	14.0	-15.5
5	3	-11	25.1	-24.8
3	3	-11	30.5	-29.5
-1	3	-11	13.8	14.4
0	2	-11	16.0	15.7
2	2	-11	16.0	16.0
4	2	-11	12.3	12.0
3	1	-11	7.0	-7.1
1	1	-11	17.5	-17.1
-1	1	-11	13.1	-13.0
0	0	-11	36.0	-35.9
2	0	-11	12.2	-11.8
-1	1	-10	16.3	-16.0
1	1	-10	10.3	-10.0
6	0	-10	28.7	29.4
4	0	-10	31.9	31.8
2	0	-10	56.1	55.6
0	0	-10	36.0	34.3
2	2	-10	14.7	-15.0
0	2	-10	13.8	13.7
-1	3	-10	10.9	10.9
5	3	-10	11.6	-11.7
4	4	-10	16.8	-16.8
1	5	-10	10.4	-10.6
0	6	-10	22.8	22.7
4	6	-10	31.1	31.0
2	6	-10	27.3	25.6
0	6	-10	27.6	27.6
-1	7	-10	13.5	-15.0
-1	9	-10	11.5	11.9
-1	11	-10	8.0	-8.0
5	9	-9	9.0	-9.2
3	9	-9	38.4	-38.0
1	9	-9	29.6	-28.9
-1	9	-9	21.0	-21.1
0	8	-9	11.5	-11.4

H	K	L	/FO/	/FC/
2	8	-9	8.2	-7.3
0	7	-9	13.0	-12.8
6	6	-9	20.6	-21.0
7	5	-9	8.5	-10.2
5	5	-9	9.6	-9.5
0	4	-9	23.0	-22.8
2	4	-9	8.3	-7.6
6	3	-9	24.5	-23.8
3	3	-9	59.0	-57.9
1	3	-9	62.0	-61.9
-1	3	-9	52.4	-51.4
2	2	-9	25.0	-24.9
6	2	-9	16.3	16.9
7	1	-9	11.9	-13.2
5	1	-9	14.5	-15.2
0	0	-9	21.0	-21.4
2	0	-9	16.6	16.3
6	0	-9	36.7	-36.7
3	1	-9	6.0	-5.5
1	1	-8	15.0	-14.6
3	1	-8	33.3	-33.5
5	1	-8	21.1	-21.4
6	0	-8	18.2	19.1
0	0	-8	10.9	-11.9
4	0	-8	9.0	-9.7
2	0	-8	33.3	32.9
0	0	-8	63.0	63.2
6	2	-8	15.8	15.1
4	2	-8	14.2	14.2
2	2	-8	23.2	23.5
-1	3	-8	14.5	-14.9
1	3	-8	16.3	-16.8
3	3	-8	49.0	49.5
5	3	-8	55.5	54.3
4	4	-8	30.9	29.9
2	4	-8	14.2	13.5
0	4	-8	13.2	-13.2
3	5	-8	30.3	-29.8
5	5	-8	18.1	-18.2
4	6	-8	21.2	-21.6
2	6	-8	26.6	25.1
0	6	-8	55.1	54.3
1	7	-8	14.6	-14.8
3	7	-8	14.8	-14.8
5	7	-8	11.1	-12.4
1	8	-8	16.4	15.8
3	8	-8	9.5	8.2
0	8	-8	7.3	-7.1
-1	9	-8	9.7	-9.8
1	9	-8	24.3	22.0

H	K	L	/FO/	/FC/
5	9	-8	29.2	30.3
4	10	-8	10.7	9.6
1	11	-8	7.3	-8.0
3	11	-8	8.9	-8.5
0	12	-8	19.5	19.8
0	12	-7	17.9	-18.2
2	12	-7	28.2	-28.5
1	11	-7	13.3	-13.5
0	10	-7	13.0	13.3
2	10	-7	15.7	16.0
5	9	-7	26.5	-25.8
1	9	-7	19.4	20.1
-1	9	-7	21.6	-20.9
0	8	-7	22.9	23.1
2	8	-7	18.6	18.2
4	8	-7	10.1	10.3
3	7	-7	15.4	-14.9
1	7	-7	28.5	-28.3
0	6	-7	47.1	-47.1
2	6	-7	59.8	-59.9
4	6	-7	22.2	-20.8
6	6	-7	14.0	16.1
3	5	-7	13.7	-13.2
1	5	-7	23.0	-22.6
-1	5	-7	23.8	-24.2
0	4	-7	40.3	39.4
2	4	-7	21.8	21.5
4	4	-7	19.9	19.6
7	3	-7	35.1	-35.8
5	3	-7	39.0	-38.5
3	3	-7	8.4	8.3
1	3	-7	21.2	21.9
-1	3	-7	32.0	-31.5
0	2	-7	33.9	33.6
2	2	-7	57.5	58.7
3	1	-7	20.4	-20.2
1	1	-7	35.9	-36.6
-1	1	-7	26.3	-25.7
0	0	-7	51.7	-51.9
2	0	-7	114.8	-115.9
4	0	-7	12.6	-12.9
6	0	-7	20.2	21.8
-1	1	-6	30.5	-30.2
1	1	-6	8.5	-8.8
3	1	-6	15.0	15.3
5	1	-6	13.7	13.5
6	0	-6	43.3	42.5
4	0	-6	93.8	93.3
2	0	-6	91.7	94.2

H	K	L	/FO/	/FC/
6	2	-6	10.1	-10.6
2	2	-6	31.6	33.5
0	2	-6	20.1	20.5
-1	3	-6	112.8	110.7
1	3	-6	46.8	48.3
3	3	-6	32.3	-33.5
7	3	-6	11.2	11.5
0	4	-6	54.7	54.9
-1	5	-6	29.3	-28.7
1	5	-6	10.2	-10.2
3	5	-6	18.2	17.8
5	5	-6	8.5	8.3
6	6	-6	22.1	22.2
4	6	-6	68.7	68.6
2	6	-6	75.3	73.8
-1	7	-6	11.8	-12.4
5	7	-6	14.3	13.5
0	8	-6	24.1	24.1
-1	9	-6	48.5	48.7
1	9	-6	20.4	20.1
0	10	-6	13.7	13.8
4	12	-6	27.4	27.5
2	12	-6	25.9	24.8
0	12	-6	12.0	13.3
1	11	-6	13.6	13.1
5	9	-5	10.2	-9.8
3	9	-5	26.3	-25.8
1	9	-5	64.5	-64.9
-1	9	-5	35.4	-35.3
1	7	-5	21.7	21.4
0	6	-5	31.8	32.2
2	6	-5	15.1	15.8
4	6	-5	8.1	-7.6
6	6	-5	17.3	-16.5
7	5	-5	10.5	-10.9
3	5	-5	16.9	16.8
-1	5	-5	5.2	5.3
0	4	-5	16.2	16.3
4	4	-5	12.3	-11.8
6	4	-5	13.2	12.6
5	3	-5	26.0	-24.6
3	3	-5	62.9	-63.5
1	3	-5	113.4	-115.2
-1	3	-5	91.0	-90.7
0	2	-5	8.7	-8.4
2	2	-5	12.5	-13.3
4	2	-5	14.8	13.7
8	2	-5	7.6	8.8
7	1	-5	11.4	-11.6

H	K	L	/FO/	/FC/
1	1	-5	10.4	9.0
0	0	-5	94.3	93.0
2	0	-5	37.2	36.7
4	0	-5	36.1	-36.9
6	0	-5	13.0	-12.7
8	0	-5	14.0	-14.7
-1	1	-4	7.4	7.4
1	1	-4	17.0	-16.8
3	1	-4	32.4	-32.9
5	1	-4	29.0	-28.5
7	1	-4	13.2	-13.5
4	0	-4	18.7	18.2
2	0	-4	76.7	78.8
0	0	-4	50.9	52.9
6	2	-4	18.6	17.7
4	2	-4	32.6	33.0
2	2	-4	22.8	-23.7
-1	3	-4	35.1	-34.7
1	3	-4	39.9	43.4
3	3	-4	27.5	28.6
5	3	-4	28.5	27.6
7	3	-4	28.5	30.3
6	4	-4	13.2	13.4
4	4	-4	13.0	12.7
2	4	-4	24.5	24.9
0	4	-4	21.4	-22.0
-1	5	-4	18.2	18.5
1	5	-4	13.8	-13.8
3	5	-4	26.8	-26.5
5	5	-4	18.8	-18.8
7	5	-4	10.4	-12.5
4	6	-4	22.8	21.4
2	6	-4	21.0	20.3
0	6	-4	61.8	61.4
3	7	-4	12.6	-13.1
5	7	-4	24.3	-23.2
6	8	-4	10.0	8.9
4	8	-4	8.9	8.9
0	8	-4	14.1	-13.2
1	9	-4	8.1	7.4
3	9	-4	12.9	13.3
5	9	-4	22.3	21.5
4	10	-4	10.4	9.8
5	11	-4	12.0	-13.0
2	12	-4	8.5	9.5
0	12	-4	20.0	20.0
3	13	-3	13.0	-12.8
1	13	-3	8.8	-9.1
0	12	-3	15.8	-15.5

Sample 1. Tas27-2Ba (continued)

H	K	L	/FO/	/FC/
3	3	10	30.6	32.4
5	3	10	18.6	17.6
4	4	10	11.5	12.1
2	4	10	9.6	9.7
3	5	10	10.6	-12.1
4	6	10	9.7	-10.3
3	9	10	17.6	18.1
1	7	11	8.4	-9.1
2	6	11	15.3	-16.9
2	4	11	7.3	7.2
5	3	11	20.4	-18.0
3	3	11	9.7	-9.7
2	2	11	20.4	20.9
2	0	11	35.0	-33.5
4	0	12	20.6	19.2
[illegible]	0	12	38.0	38.8
[illegible]	3	12	13.2	-14.0
[illegible]	5	12	8.5	7.8
[illegible]	6	12	31.2	31.5
[illegible]	0	13	12.8	-11.5
[illegible]	4	14	9.4	8.2
[illegible]	0	15	10.8	-9.9

Table 8. Observed (FO) and calculated (FC) structure factors for sample 2. Tas27-2Bb.

H	K	L	/FO/	/FC/
-1	1	-1	41.7	-45.1
-1	1	1	14.4	12.9
-1	1	2	67.9	-68.9
-1	1	3	82.6	-80.1
-1	1	4	19.5	-19.6
-1	1	5	11.8	9.7
-1	1	6	9.2	-10.2
-1	1	7	41.0	-40.7
-1	1	8	16.7	-17.2
-1	1	10	12.4	-12.2
-1	1	11	22.8	-22.5
-1	1	12	14.5	-13.9
-1	1	13	7.6	7.2
-1	1	15	19.5	-18.5
-1	1	16	13.5	-13.3
1	1	0	32.4	35.4
-1	1	9	5.1	4.9
-1	3	-1	40.2	35.9
1	3	0	53.3	-50.9
-1	3	1	116.9	-119.2
-1	3	2	97.6	96.2
-1	3	3	107.5	-109.0
-1	3	4	45.3	46.2
-1	3	5	130.2	-128.7
-1	3	6	54.2	53.5
-1	3	7	25.0	24.0
-1	3	8	18.3	-20.3
-1	3	9	74.7	-75.6
-1	3	12	50.5	50.6
-1	3	13	65.6	-64.4
-1	3	14	5.8	-5.9
-1	3	15	10.1	-9.7
-1	3	16	20.5	21.0
-1	5	-1	39.3	-40.2
1	5	0	15.4	15.9
-1	5	1	20.2	19.4
-1	5	2	30.6	-31.5
-1	5	3	46.4	-46.6
-1	5	4	15.4	-15.4
-1	5	6	12.3	-12.3
-1	5	7	27.1	-26.8
-1	5	8	6.1	-6.0
-1	5	9	8.7	8.8
-1	5	10	13.6	-13.8
-1	5	11	21.7	-22.8
-1	5	12	12.5	-12.6
-1	5	13	10.1	10.7
-1	5	14	7.6	7.0
-1	5	15	15.1	-15.4
1	7	0	29.3	30.4

H	K	L	/FO/	/FC/
-1	7	2	48.1	-49.6
-1	7	3	46.1	-47.7
-1	7	4	7.0	7.2
-1	7	5	25.8	25.3
-1	7	7	35.5	-35.6
-1	7	8	19.6	-19.4
-1	7	11	8.1	-8.2
-1	7	12	7.5	-7.9
-1	9	-1	8.1	-7.4
-1	9	0	30.8	-31.9
-1	9	1	50.8	-50.6
-1	9	2	73.0	72.9
-1	9	3	26.4	-27.0
-1	9	4	9.3	9.5
-1	9	6	85.2	-84.5
-1	9	8	27.2	26.8
-1	9	7	27.2	27.3
-1	9	9	42.2	-42.0
-1	9	12	33.9	34.4
-1	9	13	37.5	-37.4
1	11	0	17.8	17.9
-1	11	2	28.3	-28.6
-1	11	3	24.1	-24.2
-1	11	4	5.3	5.0
-1	11	5	18.9	18.8
-1	11	7	20.7	-20.5
-1	11	8	12.1	-11.9
-1	13	-1	11.9	-12.0
-1	13	0	11.1	10.8
-1	13	1	8.7	8.5
-1	13	2	8.5	-8.5
-1	13	3	14.7	-14.7
-1	13	7	11.0	-10.4
-1	13	-7	12.3	-11.5
-1	13	-6	11.3	-11.6
-1	13	-4	13.2	12.6
-1	13	-2	20.2	-19.3
-1	11	-10	14.4	-14.6
-1	11	-6	10.5	-10.3
-1	11	-3	10.7	-10.7
-1	11	-2	21.3	-21.8
-1	9	-12	6.8	-7.1
-1	9	-11	10.9	10.9
-1	9	-10	10.8	10.7
-1	9	-9	33.9	-33.1
-1	9	-8	14.3	-14.4
-1	9	-7	31.1	-30.5
-1	9	-6	68.0	67.8
-1	9	-5	47.2	-47.2
-1	9	-4	7.2	-6.9

H	K	L	/FO/	/FC/
-1	9	-3	30.3	-29.8
-1	9	-2	32.5	32.7
-1	7	-14	8.6	-8.2
-1	7	-13	12.9	14.0
-1	7	-12	6.6	6.8
-1	7	-11	13.5	-15.0
-1	7	-10	21.0	-21.7
-1	7	-9	8.0	-8.0
-1	7	-8	8.7	8.9
-1	7	-7	8.2	-8.5
-1	7	-6	16.1	-14.7
-1	7	-5	4.7	-4.2
-1	7	-3	25.4	-25.6
-1	7	-2	35.2	-35.8
-1	5	-14	11.8	-11.6
-1	5	-13	5.7	6.2
-1	5	-11	13.3	-14.1
-1	5	-10	11.9	-13.0
-1	5	-7	30.3	-30.1
-1	5	-6	34.3	-34.1
-1	5	-4	21.0	20.7
-1	5	-3	15.4	-15.6
-1	5	-2	64.5	-65.3
-1	3	-15	13.0	-11.8
-1	3	-14	18.4	17.7
-1	3	-13	46.4	-45.2
-1	3	-11	21.1	21.0
-1	3	-10	15.1	15.1
-1	3	-9	66.1	-67.6
-1	3	-8	18.4	-18.2
-1	3	-7	37.3	-39.1
-1	3	-6	131.6	131.1
-1	3	-5	104.1	-104.3
-1	3	-4	40.0	-38.2
-1	3	-3	86.2	-84.9
-1	3	-2	42.7	41.0
-1	1	-15	17.6	-17.5
-1	1	-14	13.0	-12.9
-1	1	-13	9.3	9.6
-1	1	-11	19.7	-18.7
-1	1	-10	28.6	-31.3
-1	1	-7	29.9	-30.8
-1	1	-6	34.8	-34.1
-1	1	-4	8.4	8.8
-1	1	-3	40.9	-41.2
-1	1	-2	90.0	-86.9
-1	1	-9	5.2	-5.0
0	14	4	8.8	-8.9
0	14	2	10.1	10.1
0	12	8	33.2	33.2

H	K	L	/FO/	/FC/
0	12	7	30.0	-29.6
0	12	5	20.6	20.1
0	12	4	30.2	29.7
0	12	3	23.7	-22.9
0	12	1	20.8	-21.5
0	12	0	73.4	73.7
0	10	12	7.6	7.6
0	10	11	14.4	14.5
0	10	10	7.6	7.1
0	10	9	11.3	-10.7
0	10	7	18.2	18.8
0	10	6	20.2	19.4
0	10	4	8.9	-9.0
0	10	3	7.9	8.3
0	10	2	23.9	24.2
0	10	1	4.9	4.5
0	10	0	7.1	-7.9
0	8	13	6.5	-6.2
0	8	12	13.3	13.5
0	8	11	20.7	21.7
0	8	10	6.1	5.7
0	8	9	10.3	-10.9
0	8	8	9.9	-9.9
0	8	7	30.3	30.0
0	8	6	31.9	31.8
0	8	4	17.2	-16.8
0	8	3	5.1	4.3
0	8	2	25.2	25.2
0	8	1	15.2	15.2
0	6	14	12.5	12.7
0	6	13	23.7	24.4
0	6	12	16.1	16.1
0	6	11	49.7	-51.8
0	6	10	39.3	39.2
0	6	8	70.1	70.3
0	6	7	58.4	-58.0
0	6	6	8.8	-8.7
0	6	5	36.4	37.7
0	6	4	70.3	70.1
0	6	3	28.8	-30.8
0	6	2	11.2	13.4
0	6	1	54.1	-55.9
0	4	15	6.5	6.3
0	4	13	6.8	-6.7
0	4	12	23.3	23.8
0	4	11	31.8	33.2
0	4	10	9.1	9.4
0	4	9	28.5	-29.0
0	4	8	15.0	-15.3
0	4	7	47.3	46.3

H	K	L	/FO/	/FC/
0	4	6	63.8	62.9
0	4	5	18.5	18.9
0	4	4	23.9	-23.2
0	4	3	14.8	-15.5
0	4	2	29.7	31.3
0	4	1	42.0	43.6
0	4	0	44.5	44.8
0	2	16	8.2	8.0
0	2	15	20.0	20.3
0	2	13	10.9	-10.6
0	2	12	7.5	6.9
0	2	11	21.4	21.6
0	2	10	17.8	18.0
0	2	8	4.5	5.0
0	2	7	38.7	38.7
0	2	6	23.5	23.5
0	2	5	9.8	-7.8
0	2	3	64.1	60.9
0	2	2	85.5	84.4
0	2	1	11.8	14.9
0	2	0	38.1	-39.7
0	0	16	29.4	-29.9
0	0	13	34.7	34.4
0	0	12	40.9	39.7
0	0	11	50.8	-49.3
0	0	10	47.1	45.3
0	0	9	24.9	-26.9
0	0	8	73.2	75.7
0	0	7	58.8	-58.4
0	0	6	40.4	40.4
0	0	5	105.0	103.1
0	0	4	56.0	57.5
0	0	3	107.0	-109.4
0	0	2	15.9	-15.9
0	0	1	50.4	-48.9
0	12	-9	5.7	-4.7
2	14	2	8.7	8.4
2	14	1	13.2	13.1
2	14	-1	6.2	-6.5
2	12	8	23.2	22.6
2	12	6	11.5	-13.1
2	12	5	14.2	-13.9
2	12	4	50.5	49.6
2	12	3	15.9	-15.9
2	12	2	10.9	10.5
2	12	1	43.7	-42.4
2	12	0	39.9	40.0
2	12	-1	23.8	24.3
2	10	10	10.7	11.1
2	10	8	13.2	-13.4

H	K	L	/FO/	/FC/
2	10	6	27.6	26.3
2	10	5	12.3	11.8
2	10	4	9.5	-9.4
2	10	3	10.8	-11.2
2	10	2	14.2	14.5
2	10	1	18.8	20.0
2	10	-1	5.7	-6.3
2	8	11	11.1	11.6
2	8	10	11.4	11.9
2	8	8	11.2	-11.4
2	8	7	9.2	9.0
2	8	6	26.9	27.2
2	8	5	11.3	10.8
2	8	4	16.1	-14.0
2	8	3	4.7	-5.4
2	8	2	24.7	25.5
2	8	1	30.5	30.7
2	8	-1	10.9	-12.2
2	6	12	55.8	56.1
2	6	11	28.0	-28.7
2	6	9	7.1	-7.4
2	6	8	39.5	39.2
2	6	6	9.9	-10.6
2	6	5	14.9	-14.8
2	6	4	105.8	105.9
2	6	3	40.4	-42.1
2	6	2	20.9	21.1
2	6	1	87.5	-87.6
2	6	0	98.8	100.9
2	6	-1	66.3	65.8
2	4	14	14.8	15.2
2	4	11	11.2	11.7
2	4	10	14.8	14.8
2	4	8	5.8	-6.5
2	4	7	18.0	18.2
2	4	6	40.1	39.5
2	4	5	7.8	7.6
2	4	4	22.0	-20.2
2	4	2	55.7	54.9
2	4	1	56.2	56.2
2	4	-1	26.7	-27.4
2	2	13	10.5	-10.4
2	2	11	30.3	31.1
2	2	10	27.2	28.2
2	2	8	33.3	-33.5
2	2	6	59.2	60.0
2	2	5	50.4	51.7
2	2	3	28.3	-28.6
2	2	1	39.2	39.3
2	2	0	45.0	44.5

H	K	L	/FO/	/FC/
4	0	-6	108.1	107.1
4	0	-7	15.6	-15.0
4	0	-8	10.1	-10.5
4	0	-10	38.5	39.4
4	0	-11	7.5	-7.6
4	0	-13	28.8	-28.7
4	0	-14	57.2	57.1
4	2	-2	23.3	-24.4
4	2	-3	16.9	17.7
4	2	-4	36.1	37.8
4	2	-5	16.0	15.9
4	2	-7	8.1	7.4
4	2	-8	15.7	16.4
4	2	-10	5.4	-6.2
4	2	-11	16.5	15.2
4	2	-12	23.7	22.1
4	2	-13	8.4	8.7
4	2	-14	13.4	-13.5
4	2	-15	7.2	-8.6
4	4	-2	8.4	8.6
4	4	-3	24.6	24.2
4	4	-4	14.5	14.6
4	4	-5	13.2	-14.0
4	4	-7	23.2	23.6
4	4	-8	36.1	36.6
4	4	-10	19.9	-20.2
4	4	-12	19.8	19.0
4	4	-13	19.5	19.3
4	4	-15	7.4	-8.0
4	6	-2	50.4	50.7
4	6	-3	73.0	-73.2
4	6	-4	27.3	27.0
4	6	-5	9.3	-9.5
4	6	-6	86.7	85.1
4	6	-7	27.5	-27.2
4	6	-8	26.4	-27.4
4	6	-10	41.3	42.4
4	6	-11	5.7	6.4
4	6	-13	33.8	-34.7
4	6	-14	38.6	37.6
4	8	-3	17.3	16.0
4	8	-4	11.9	11.5
4	8	-5	6.0	-5.8
4	8	-6	5.3	-5.8
4	8	-7	13.9	14.1
4	8	-8	22.3	21.7
4	8	-10	13.8	-14.8
4	8	-12	13.6	13.6
4	10	-2	5.7	-6.0
4	10	-3	11.5	11.0
4	10	-4	14.5	14.6
4	10	-7	5.6	5.8
4	10	-8	15.3	14.5
4	10	-10	8.0	-8.4
4	12	-2	29.2	28.4
4	12	-3	40.5	-40.0
4	12	-4	9.2	8.6
4	12	-5	10.7	-10.3
4	12	-6	44.4	44.7
4	12	-7	12.5	-12.6
5	1	-1	7.9	7.6
5	1	0	21.6	-20.8
5	1	1	24.2	-24.1
5	1	3	6.0	5.7
5	1	4	12.2	-11.6
5	1	5	23.1	-22.9
5	1	7	11.5	12.0
5	1	8	5.4	-5.5
5	1	9	16.1	-16.5
5	1	10	12.4	-11.4
5	1	11	6.4	6.6
5	3	-1	52.0	-51.3
5	3	0	73.6	73.3
5	3	1	26.8	-26.8
5	3	2	9.0	9.6
5	3	3	81.7	-84.4
5	3	4	26.4	27.0
5	3	5	27.0	26.8
5	3	7	42.8	-42.2
5	3	8	6.0	-5.8
5	3	10	35.3	34.1
5	3	11	38.7	-37.3
5	5	0	20.8	-20.6
5	5	1	15.7	-16.8
5	5	2	5.7	5.8
5	5	3	8.2	8.7
5	5	4	11.1	-12.3
5	5	5	22.1	-22.9
5	5	7	13.4	13.8
5	5	9	13.0	-12.9
5	5	10	12.1	-12.1
5	7	-1	14.8	14.8
5	7	0	8.9	-9.8
5	7	1	21.1	-20.9
5	7	5	10.0	-10.3
5	7	8	9.0	-8.5
5	7	9	12.8	-13.8
5	9	-1	39.9	-40.4
5	9	0	41.7	42.6
5	9	1	11.3	-10.4
5	9	2	17.2	16.0
5	9	3	49.9	-49.6
5	9	4	13.8	14.0
5	9	5	11.9	12.7
5	9	7	21.5	-22.8
5	11	-1	12.3	12.2
5	11	1	11.8	-11.8
5	11	-7	7.6	7.3
5	11	-6	12.4	12.9
5	11	-4	20.3	-20.8
5	11	-3	10.9	-11.7
5	11	-2	9.1	8.6
5	9	-9	15.3	-14.0
5	9	-8	45.8	45.5
5	9	-7	39.3	-38.4
5	9	-6	10.1	-10.4
5	9	-5	14.6	-14.2
5	9	-4	32.0	31.9
5	9	-2	24.8	-24.1
5	7	-9	20.3	-18.3
5	7	-8	15.8	-16.4
5	7	-7	7.1	7.6
5	7	-6	19.1	18.9
5	7	-5	5.8	-5.3
5	7	-4	29.2	-30.6
5	7	-3	19.4	-19.4
5	7	-2	13.3	13.0
5	5	-13	13.9	-14.3
5	5	-12	10.8	-11.1
5	5	-10	11.1	11.3
5	5	-9	12.0	-12.0
5	5	-8	23.8	-23.6
5	5	-6	10.9	10.6
5	5	-4	22.5	-22.8
5	5	-3	13.0	-13.3
5	5	-2	6.0	6.7
5	3	-14	6.4	-7.2
5	3	-13	19.0	19.3
5	3	-12	20.2	20.5
5	3	-11	33.9	-33.7
5	3	-10	14.8	-14.6
5	3	-9	30.4	-31.9
5	3	-8	67.1	68.6
5	3	-7	45.8	-47.3
5	3	-6	6.7	-6.9
5	3	-5	31.4	-30.2
5	3	-4	34.1	33.4
5	3	-3	8.0	-7.8
5	3	-2	32.4	-31.5
5	1	-13	14.5	-13.8
5	1	-12	9.6	-9.7
5	1	-10	8.6	8.3
5	1	-9	18.5	-18.6
5	1	-8	26.1	-26.0
5	1	-6	16.7	16.1
5	1	-5	4.7	-4.1
5	1	-4	33.0	-33.0
5	1	-3	21.4	-21.0
5	1	-2	9.8	9.8
6	10	2	9.6	-8.9
6	10	0	15.2	14.5
6	8	5	14.0	14.8
6	8	4	6.6	6.4
6	8	3	9.1	-8.5
6	8	2	9.8	-10.1
6	8	1	11.2	10.8
6	8	0	22.0	20.0
6	6	6	30.9	33.0
6	6	5	29.4	-30.1
6	6	3	20.0	19.8
6	6	2	31.8	30.3
6	6	1	24.1	-23.5
6	6	-1	21.6	-21.5
6	4	5	21.4	21.1
6	4	4	8.8	9.0
6	4	3	13.1	-14.2
6	4	2	12.7	-13.5
6	4	1	15.3	15.3
6	4	0	32.9	32.5
6	4	-1	7.6	7.1
6	2	9	14.6	15.4
6	2	8	6.1	6.2
6	2	7	10.7	-11.3
6	2	6	8.3	-8.1
6	2	5	18.0	18.0
6	2	4	17.5	18.4
6	2	2	8.9	-9.5
6	2	1	6.7	6.1
6	2	0	18.4	17.6
6	0	9	43.9	-43.8
6	0	8	17.3	18.5
6	0	6	49.8	52.0
6	0	5	31.3	-31.5
6	0	4	11.2	-11.7
6	0	3	9.5	9.9
6	0	2	35.8	34.4
6	0	1	18.8	-17.7
6	0	0	12.7	12.2
6	0	-1	23.2	-22.1
6	0	-2	80.1	80.7
6	0	-3	42.6	-43.0
6	0	-4	6.3	-6.8
6	0	-5	16.3	-16.0
6	0	-6	55.4	54.6
6	0	-7	25.2	26.4
6	0	-8	14.4	-15.3
6	0	-9	48.4	-49.1
6	0	-10	40.6	40.2
6	0	-11	5.6	6.2
6	0	-12	33.5	33.4
6	0	-13	36.3	-35.4
6	2	-3	9.5	9.1
6	2	-4	22.3	22.4
6	2	-5	5.6	5.3
6	2	-6	13.8	-14.3
6	2	-8	20.3	20.5
6	2	-9	22.6	22.2
6	2	-11	13.1	-12.8
6	2	-13	14.5	13.6
6	4	-2	18.5	-17.7
6	4	-3	8.0	-8.5
6	4	-4	18.4	17.5
6	4	-5	17.7	16.9
6	4	-8	7.3	7.4
6	4	-12	12.2	12.7
6	6	-2	75.0	74.2
6	6	-3	21.9	-21.8
6	6	-5	23.6	-23.7
6	6	-6	31.4	30.7
6	6	-7	20.5	20.1
6	6	-9	28.7	-30.3
6	6	-10	32.3	33.5
6	8	-2	13.8	-13.8
6	8	-4	14.1	13.5
6	8	-5	10.8	10.8
6	8	-8	6.6	6.2
6	8	-9	9.7	8.5
6	10	-2	6.8	-7.1
6	10	-4	10.2	10.3
7	1	-1	6.5	-5.7
7	1	0	16.7	-16.7
7	1	2	6.3	6.3
7	1	4	13.3	-13.5
7	1	5	6.7	-8.6
7	1	6	8.7	8.8
7	3	0	30.2	32.4
7	3	1	12.5	-14.4
7	3	2	8.2	-10.1
7	3	3	37.8	-38.1
7	3	4	44.9	45.1
7	3	5	14.9	-13.8
7	5	0	15.5	-16.1
7	5	4	8.6	-9.4
7	7	-1	7.6	-7.3
7	7	0	9.5	-9.7
7	7	2	7.6	8.1
7	7	-6	7.4	6.9
7	7	-5	5.6	-6.8
7	7	-4	9.5	-9.4
7	5	-10	5.9	-6.0
7	5	-9	14.3	-15.0
7	5	-7	12.7	12.5
7	5	-5	17.7	-16.1
7	5	-4	17.4	-17.9
7	5	-2	12.5	12.6
7	3	-11	23.3	-23.3
7	3	-9	13.0	12.8
7	3	-8	14.5	14.6
7	3	-7	47.3	-50.5
7	3	-6	16.1	16.2
7	3	-5	10.5	-10.3
7	3	-4	43.7	43.0
7	3	-3	42.7	-40.5
7	3	-2	23.1	-24.2
7	1	-11	8.2	8.2
7	1	-9	18.8	-18.2
7	1	-7	10.5	11.1
7	1	-6	6.0	6.0
7	1	-5	16.2	-15.9
7	1	-4	18.0	-17.9
7	1	-2	10.4	10.7
8	4	0	6.9	8.2
8	2	2	13.5	-13.7
8	2	0	17.2	15.9
8	2	-1	19.8	18.1
8	0	3	13.5	-12.7
8	0	2	45.5	44.7
8	0	1	11.3	-10.3
8	0	0	9.9	8.3
8	0	-1	41.3	-40.4
8	0	-2	29.9	29.2
8	0	-3	20.8	20.3
8	0	-5	23.2	-23.2
8	0	-6	9.9	10.3
8	0	-8	28.6	28.7
8	2	-3	13.8	-13.7
8	2	-5	13.2	13.0
8	2	-6	6.6	6.8
8	4	-4	9.3	8.5
8	4	-5	12.7	12.7

Table 8. Observed (FO) and calculated (FC) structure factors for sample 3. Tag15-4.

H	K	L	/FO/	/FC/
0	12	-3	19.0	-18.6
2	12	-3	24.1	-24.1
4	12	-3	26.6	-27.3
1	11	-3	21.2	-20.2
2	10	-3	14.2	14.6
3	9	-3	15.2	-14.3
1	9	-3	27.2	-25.7
-1	9	-3	29.6	-28.3
-3	9	-3	45.9	-45.5
-5	9	-3	37.2	-38.6
2	8	-3	24.5	24.1
3	7	-3	25.3	-24.4
1	7	-3	42.4	-42.8
-1	7	-3	24.1	-23.1
-3	7	-3	11.7	10.1
-6	6	-3	13.8	12.4
-2	6	-3	43.3	-42.6
0	6	-3	33.4	-35.7
2	6	-3	65.7	-66.0
4	6	-3	62.6	-64.2
3	5	-3	52.5	-53.1
1	5	-3	43.5	-44.8
-1	5	-3	16.7	-16.9
2	4	-3	46.4	47.0
4	4	-3	23.5	23.6
7	3	-3	33.8	-34.8
3	3	-3	20.4	-21.2
1	3	-3	110.1	-111.9
-1	3	-3	89.1	-87.6
-3	3	-3	72.8	-70.8
-5	3	-3	76.7	-75.9
-7	3	-3	32.0	-32.6
-4	2	-3	22.2	-21.8
-2	2	-3	24.5	-25.7
0	2	-3	59.3	60.4
2	2	-3	15.7	17.3
4	2	-3	15.2	16.9
5	1	-3	20.1	-19.7
3	1	-3	61.0	-63.4
1	1	-3	75.9	-78.2
-1	1	-3	40.3	-40.2
-3	1	-3	53.2	-54.4
0	0	-3	116.7	-115.6
2	0	-3	46.9	-49.1
4	0	-3	83.6	-84.6
6	0	-3	38.5	-38.1
5	3	-3	14.0	-13.8
-3	3	-2	34.8	36.6
-1	3	-2	47.9	48.8
1	3	-2	98.4	100.6
3	3	-2	56.4	58.0
5	3	-2	22.7	-22.5
7	3	-2	15.4	-15.3
4	2	-2	20.0	-20.8
2	2	-2	40.4	41.7
0	2	-2	79.6	80.6
-3	1	-2	37.1	-37.9
1	1	-2	85.8	-85.6
1	1	-2	63.4	-64.9
3	1	-2	19.0	-19.5
6	0	-2	72.0	71.9
4	0	-2	98.8	100.0
2	0	-2	24.5	-23.4
-2	0	-2	113.6	113.0
-4	0	-2	27.3	27.7
6	0	-2	33.5	32.4
8	0	-2	33.9	34.3
1	2	-2	11.1	12.2
0	4	-2	13.9	-12.7
2	4	-2	12.3	13.3
0	4	-2	28.4	29.9
-2	4	-2	50.8	52.1
-3	5	-2	30.4	-30.4
-1	5	-2	58.4	-60.5
1	5	-2	28.1	-28.8
3	5	-2	16.4	-16.4
6	6	-2	59.5	60.2
4	6	-2	49.0	49.1
0	6	-2	19.4	19.7
-2	6	-2	25.3	24.6
-4	6	-2	32.2	30.0
-6	6	-2	26.7	26.4
-3	7	-2	14.7	-15.0
-1	7	-2	33.0	-33.9
1	7	-2	44.1	-45.7
2	8	-2	13.0	11.0
0	8	-2	24.6	23.7
-2	8	-2	23.2	23.4
-3	9	-2	16.4	15.9
-1	9	-2	31.9	31.0
1	9	-2	64.7	62.8
3	9	-2	18.9	19.0
0	10	-2	20.0	20.0
-1	11	-2	17.5	-16.1
1	11	-2	22.7	-20.7
-1	13	-2	15.4	-14.5
-4	12	-1	16.2	-16.6
-2	12	-1	32.7	-31.1
-4	10	-1	16.9	15.5
-2	10	-1	16.6	16.5
5	9	-1	32.9	-33.5
3	9	-1	68.2	-68.2
1	9	-1	49.9	-47.7
-1	9	-1	12.6	-12.3
-4	8	-1	15.9	16.6
-2	8	-1	26.7	25.6
0	8	-1	14.0	12.6
2	8	-1	10.2	-10.2
-3	7	-1	30.4	-30.3
-5	7	-1	17.1	-17.6
-6	6	-1	21.0	-20.5
-4	6	-1	33.1	-32.1
-2	6	-1	84.3	-83.1
0	6	-1	56.2	-56.6
2	6	-1	53.9	53.3
4	6	-1	23.9	23.0
6	6	-1	19.1	-18.4
3	5	-1	21.4	22.7
1	5	-1	15.9	16.6
-1	5	-1	38.8	-39.0
-3	5	-1	27.0	-27.9
-5	5	-1	16.7	-15.2
-6	4	-1	14.1	14.0
-4	4	-1	20.1	20.5
-2	4	-1	53.0	53.5
0	4	-1	40.9	41.8
2	4	-1	23.2	-24.1
5	3	-1	51.3	-50.7
3	3	-1	155.0	-155.4
1	3	-1	124.2	-123.7
-1	3	-1	25.0	23.5
-3	3	-1	20.3	-20.9
-5	3	-1	29.4	-28.5
-7	3	-1	15.0	-14.7
-4	2	-1	52.4	51.8
-2	2	-1	36.1	37.1
0	2	-1	11.1	12.0
2	2	-1	41.5	42.3
4	2	-1	13.3	-14.2
3	1	-1	21.4	23.2
1	1	-1	13.7	12.4
-1	1	-1	40.3	-39.7
-3	1	-1	40.8	-41.7
-5	1	-1	21.7	-22.1
-6	0	-1	19.8	-18.4
-4	0	-1	68.0	-68.3
-2	0	-1	101.3	-101.8
0	0	-1	64.7	-64.3
2	0	-1	40.4	39.5
4	0	-1	55.1	54.1
6	0	-1	20.8	-20.9
8	0	-1	29.5	-30.2
7	3	0	26.4	26.6
5	3	0	67.1	65.7
3	3	0	57.3	57.6
1	3	0	40.1	-39.6
6	2	0	15.1	15.3
4	2	0	33.9	34.2
2	2	0	43.7	43.4
0	2	0	32.4	-33.1
8	2	0	12.4	11.9
5	1	0	19.0	-18.9
1	1	0	28.6	28.8
7	1	0	13.6	-13.3
6	0	0	16.7	16.4
4	0	0	12.4	10.4
2	0	0	125.0	125.4
6	4	0	26.1	26.0
4	4	0	19.0	19.1
0	4	0	42.0	42.7
5	5	0	17.0	-17.4
3	5	0	11.0	10.5
1	5	0	14.6	14.6
4	6	0	12.9	13.3
2	6	0	98.3	98.1
0	6	0	153.4	152.8
1	7	0	23.9	25.1
4	8	0	15.4	13.8
6	8	0	16.5	15.3
5	9	0	31.9	32.5
3	9	0	37.1	35.4
1	9	0	23.2	-23.2
1	11	0	12.7	13.0
2	12	0	30.3	31.8
0	12	0	56.9	56.1
-3	7	1	10.1	10.3
-5	7	1	12.3	10.6
5	3	2	15.1	12.7
2	10	2	12.6	13.0
-3	13	3	15.4	-14.4
-5	7	3	15.9	-15.9
-5	5	3	12.7	-12.4
0	4	3	10.2	-11.3
-7	3	4	35.7	33.8
-5	3	4	32.5	32.3
-3	3	4	34.4	36.6
-1	3	4	52.1	54.0
1	3	4	29.4	-28.4
3	3	4	29.9	-29.2
5	3	4	24.6	23.9
7	3	4	32.1	33.6
-2	2	4	21.4	-21.4
-4	2	4	33.5	35.1
-6	2	4	19.8	19.6
-5	1	4	29.6	-29.8
-3	1	4	34.1	-35.3
-1	1	4	20.8	-19.4
4	0	4	88.6	86.0
2	0	4	131.8	129.9
0	0	4	66.2	63.4
-2	0	4	87.2	87.7
-4	0	4	26.7	26.0
-7	1	4	16.7	-14.7
2	4	4	20.1	-19.6
0	4	4	21.5	-22.8
-2	4	4	26.6	26.0
-4	4	4	14.5	14.1
-6	4	4	15.7	15.1
-5	5	4	19.0	-19.2
-3	5	4	28.0	-28.2
-1	5	4	16.3	-15.1
1	5	4	18.1	19.3
4	6	4	43.8	44.7
2	6	4	100.4	99.0
0	6	4	69.8	69.9
-2	6	4	28.3	26.4
-4	6	4	28.3	27.2
-5	7	4	25.8	-25.2
-3	7	4	13.8	-14.7
2	8	4	11.8	-9.8
0	8	4	13.9	-11.3
-4	8	4	13.7	11.6
-5	9	4	25.9	25.1
-3	9	4	18.2	17.2
-1	9	4	13.0	11.3
3	9	4	17.5	-18.2
4	12	4	20.8	21.0
2	12	4	35.0	37.3
0	12	4	25.3	24.6
1	9	5	43.5	-43.0
-1	9	5	73.9	-72.7
-3	9	5	32.4	-30.8
-5	9	5	13.5	-13.3
-1	7	5	22.6	21.9
-6	6	5	21.2	-20.3
-4	6	5	11.3	-11.9
0	6	5	30.4	29.6
2	6	5	15.4	-15.1
4	6	5	57.1	-56.3
6	6	5	22.7	-23.9
5	5	5	19.0	-19.0
-3	5	5	15.4	14.5
-6	4	5	13.9	14.0
0	4	5	16.9	17.5
4	4	5	31.4	31.1
5	3	5	17.7	16.2
1	3	5	106.8	-106.7
-1	3	5	127.2	-129.1
-3	3	5	69.6	-71.1
-5	3	5	31.5	-30.3
-4	2	5	15.6	15.7
-2	2	5	11.9	-12.3
2	2	5	46.5	47.3
4	2	5	24.8	24.0
5	1	5	18.8	-19.4
3	1	5	17.2	-17.4
-3	1	5	12.2	12.3
-8	0	5	17.2	-18.0
-6	0	5	17.2	-17.2
-4	0	5	42.4	-43.5
-2	0	5	29.6	29.3
0	0	5	92.8	90.9
2	0	5	54.2	-54.5
4	0	5	67.4	-66.1
6	0	5	26.5	-27.4
-7	1	5	12.2	-13.0
6	2	5	14.2	14.3
-3	3	6	29.3	-29.9
-1	3	6	51.9	53.9
1	3	6	124.8	124.0
3	3	6	57.4	56.0
4	2	6	25.4	26.2
2	2	6	55.1	55.2
0	2	6	20.7	21.2
-2	2	6	32.3	33.0
-3	1	6	15.0	14.4
1	1	6	32.1	-32.2
3	1	6	21.9	-22.1
6	0	6	41.1	42.1
4	0	6	30.9	30.3
2	0	6	14.6	-15.4
0	0	6	49.8	48.1
-2	0	6	105.2	107.3
-4	0	6	101.4	101.4
-6	0	6	49.1	48.1
-7	3	6	15.5	14.6
4	4	6	16.4	15.6
2	4	6	35.9	34.7
0	4	6	55.4	56.2
-3	5	6	17.8	18.1

Table 8. Observed (FO) and calculated (FC) structure factors for sample 4. Tag15-3.

H	K	L	/FO/	/FC/
-1	1	-1	37.9	-38.1
1	1	-1	12.5	12.2
3	1	-1	21.6	22.3
8	0	-1	21.6	-22.2
6	0	-1	17.8	-17.3
4	0	-1	52.9	51.8
2	0	-1	39.4	38.7
0	0	-1	57.6	-58.7
4	2	-1	13.5	-12.5
2	2	-1	41.2	40.5
0	2	-1	11.8	12.1
-1	3	-1	25.4	24.5
1	3	-1	118.5	-119.6
3	3	-1	150.1	-148.4
5	3	-1	44.0	-44.2
2	4	-1	23.0	-23.0
0	4	-1	39.2	40.2
-1	5	-1	36.6	-37.8
1	5	-1	15.9	17.0
3	5	-1	21.7	22.1
6	6	-1	14.1	-14.6
4	6	-1	21.6	19.7
2	6	-1	51.8	50.8
0	6	-1	53.5	-53.0
5	7	-1	10.9	9.5
0	8	-1	12.4	12.2
-1	9	-1	11.2	-11.8
1	9	-1	44.0	-42.5
3	9	-1	56.5	-58.7
5	9	-1	27.8	-27.9
0	12	0	45.0	47.3
1	11	0	13.0	12.0
5	9	0	26.8	25.8
3	9	0	32.0	31.6
1	9	0	18.1	-19.8
1	7	0	23.4	24.4
0	6	0	147.7	146.3
2	6	0	93.5	91.8
4	6	0	11.5	11.1
5	5	0	15.3	-14.5
3	5	0	11.5	9.9
1	5	0	13.8	15.0
0	4	0	40.4	40.3
4	4	0	16.8	16.9
6	4	0	19.2	21.2
7	3	0	18.9	19.8
5	3	0	57.0	56.3
3	3	0	54.5	52.6
1	3	0	39.7	-38.3
0	2	0	32.4	-32.6

H	K	L	/FO/	/FC/
2	2	0	42.3	41.3
2	2	0	30.7	30.5
2	2	0	14.1	12.3
1	1	0	16.3	-16.7
1	1	0	27.3	27.9
0	0	0	120.1	120.7
0	0	0	8.7	7.5
0	0	0	13.7	13.4
1	1	1	37.3	-39.1
1	1	1	17.3	-19.0
0	1	1	14.6	-13.4
0	1	1	61.6	-60.1
0	1	1	99.1	-98.0
2	1	1	44.4	46.0
2	1	1	34.6	35.0
3	1	1	18.9	-16.6
3	1	1	24.1	-25.0
4	1	1	18.8	18.3
4	1	1	50.4	50.2
5	1	1	24.4	-25.0
5	1	1	13.4	-12.5
6	1	1	13.9	-15.3
6	1	1	27.2	-27.2
6	1	1	78.6	-76.8
7	1	1	27.2	-26.7
7	1	1	15.7	-14.3
8	1	1	14.4	13.2
8	1	1	23.5	22.4
10	1	1	13.3	12.4
11	1	1	12.4	-12.7
12	1	1	14.1	-12.7
12	1	1	27.1	-26.0
13	2	2	12.6	-11.7
11	2	2	19.6	-18.6
8	2	2	17.3	16.7
9	2	2	11.7	10.7
9	2	2	12.0	12.4
9	2	2	28.2	27.1
9	2	2	57.6	57.0
8	2	2	22.0	21.0
8	2	2	20.1	19.6
7	2	2	12.2	-12.4
7	2	2	31.0	-31.0
7	2	2	42.0	-43.3
6	2	2	17.4	16.9
6	2	2	22.3	21.8
6	2	2	25.7	25.6
6	2	2	18.5	18.9
5	2	2	27.6	-27.4
5	2	2	54.7	-56.2

H	K	L	/FO/	/FC/
-1	5	2	27.0	-26.9
0	4	2	25.6	26.0
2	4	2	47.5	47.2
3	3	2	31.6	30.8
1	3	2	45.1	46.5
-1	3	2	95.2	96.9
0	2	2	74.4	77.3
4	2	2	9.5	9.9
3	1	2	34.1	-34.3
1	1	2	80.4	-81.5
-1	1	2	60.1	-62.2
2	0	2	104.6	103.6
4	0	2	24.6	23.7
6	0	2	23.8	24.3
8	0	2	22.9	22.0
-1	1	3	73.3	-75.2
1	1	3	37.6	-37.1
4	0	3	9.6	8.1
2	0	3	48.0	-49.3
0	0	3	110.7	-110.7
4	2	3	18.5	-18.7
2	2	3	24.7	-24.8
0	2	3	55.4	56.6
-1	3	3	106.4	-106.8
1	3	3	83.3	-82.2
3	3	3	62.0	-60.6
5	3	3	56.9	-59.1
7	3	3	22.4	-22.4
0	4	3	10.7	-11.7
-1	5	3	41.0	-41.8
1	5	3	15.7	-15.7
2	6	3	38.8	-38.5
0	6	3	31.4	-32.7
-1	7	3	39.0	-40.0
1	7	3	22.0	-20.9
-1	9	3	25.0	-23.8
1	9	3	27.1	-25.6
3	9	3	37.8	-37.2
5	9	3	26.9	-27.9
-1	11	3	17.0	-17.1
2	12	3	11.7	-10.8
0	12	3	14.3	-16.1
-1	13	3	8.4	-8.4
0	12	4	20.2	20.4
2	12	4	27.6	28.8
4	12	4	15.8	15.0
3	9	4	13.4	-13.8
0	8	4	11.1	-10.1
0	6	4	64.3	63.1
2	6	4	86.4	85.2

H	K	L	/FO/	/FC/
4	6	4	34.3	35.7
1	5	4	17.5	18.4
-1	5	4	13.7	-14.5
0	4	4	20.7	-22.3
2	4	4	17.9	-17.3
7	3	4	20.6	22.2
5	3	4	17.2	17.9
3	3	4	26.6	-26.6
1	3	4	27.4	-26.7
-1	3	4	48.6	50.0
-1	1	4	18.3	-18.4
0	0	4	58.8	58.4
2	0	4	116.6	117.3
4	0	4	70.7	70.1
3	1	5	14.8	-13.8
5	1	5	13.9	-13.7
6	0	5	17.3	-18.6
4	0	5	53.6	-53.8
2	0	5	45.2	-45.6
0	0	5	88.1	87.0
-1	1	5	9.0	9.5
4	2	5	19.3	19.3
2	2	5	39.7	40.9
-1	3	5	122.0	-122.8
1	3	5	99.3	-96.9
5	3	5	12.6	13.2
4	4	5	24.6	24.1
0	4	5	15.9	15.8
5	5	5	12.1	-12.9
6	6	5	16.3	-15.3
4	6	5	43.4	-43.5
2	6	5	12.6	-12.5
0	6	5	28.2	27.3
-1	7	5	19.5	20.6
3	7	5	11.9	-11.9
-1	9	5	64.7	-64.2
1	9	5	37.4	-36.1
8	10	6	13.3	12.1
2	10	6	17.2	15.1
3	9	6	30.3	28.9
1	9	6	45.0	45.5
-1	9	6	18.8	19.8
0	8	6	23.1	23.4
2	8	6	18.0	18.4
3	7	6	16.5	-16.1
1	7	6	12.2	-10.9
4	6	6	19.5	19.9
6	6	6	16.3	16.8

H	K	L	/FO/	/FC/
5	6		25.8	-25.7
5	6		8.8	-9.7
4	6		50.0	50.8
4	6		30.2	29.6
3	6		45.4	46.0
3	6		114.7	113.2
3	6		48.5	49.9
2	6		19.5	20.3
2	6		48.2	47.2
2	6		18.8	19.2
1	6		18.4	-17.2
1	6		28.6	-28.0
0	6		42.2	41.6
0	6		15.8	-16.7
0	6		23.1	24.2
0	6		27.3	27.9
1	7		33.6	-34.6
1	7		24.6	-24.2
0	7		57.1	-56.9
2	7		31.2	32.1
3	7		14.5	15.8
3	7		33.6	-33.1
3	7		49.6	-49.6
3	7		22.3	-23.2
4	7		13.2	13.8
4	7		38.0	38.4
5	7		22.7	-22.1
5	7		21.7	-22.7
6	7		50.0	-48.0
7	7		25.0	-25.6
8	7		18.7	20.1
9	7		14.9	13.3
9	7		19.5	-21.2
9	7		20.4	-22.8
11	7		13.8	-12.8
12	7		16.1	-17.2
12	8		17.4	18.2
7	8		15.7	-16.0
6	8		52.2	52.7
6	8		26.9	26.6
6	8		18.4	18.4
4	8		10.8	-10.5
2	8		23.0	-22.0
2	8		15.0	-15.7
0	8		65.8	65.1
0	8		49.7	53.9
0	8		21.9	21.5
0	8		12.8	11.1

H	K	L	/FO/	/FC/
3	1	9	12.4	-10.7
6	0	9	18.5	-17.5
0	0	9	25.2	-25.4
-1	3	9	63.0	-61.1
1	3	9	51.2	-50.2
3	3	9	27.3	-28.0
0	4	9	20.4	-20.1
-1	9	9	25.2	-27.7
1	9	9	19.2	-21.0
3	9	9	16.1	-18.0
1	9	10	11.6	10.0
1	7	10	13.7	-12.3
0	6	10	29.5	30.3
5	3	10	17.6	16.5
3	3	10	29.7	29.4
1	3	10	10.4	9.5
0	2	10	11.2	11.4
2	2	10	16.9	15.9
3	1	10	11.3	-11.6
1	1	10	14.1	-13.3
0	0	10	40.7	39.3
-1	1	11	15.8	-15.4
1	1	11	11.4	-11.6
2	0	11	34.4	-32.9
0	0	11	37.9	-36.4
2	2	11	17.5	17.3
0	2	11	14.4	14.4
1	3	11	11.6	11.5
5	3	11	16.1	-15.4
0	4	11	18.5	20.5
-1	5	11	13.7	-15.0
2	6	11	16.0	-18.2
0	6	11	31.3	-32.1
0	8	11	12.9	11.4
-1	9	12	19.1	19.4
0	6	12	11.3	10.1
2	6	12	25.8	27.9
0	4	12	14.1	14.3
-1	3	12	37.0	36.8
-1	1	12	11.5	-10.2
0	0	12	26.3	24.4
2	0	12	36.1	35.7
4	0	12	18.3	17.6
0	0	13	18.9	17.5
-1	3	13	39.7	-39.9
1	3	13	24.1	-25.4
-1	9	13	16.9	-18.9

Table 8. Observed (FO) and calculated (FC) structure factors for sample 5. Tpg63-2B.

H	K	L	/FO/	/FC/
-2	12	-3	13.2	-13.3
0	12	-3	19.8	-19.1
2	12	-3	23.8	-23.5
4	12	-3	25.8	-26.3
3	11	-3	12.4	-11.5
1	11	-3	19.1	-18.2
-1	11	-3	8.6	-9.3
2	10	-3	12.2	12.4
3	9	-3	15.9	-14.8
1	9	-3	27.3	-26.2
-1	9	-3	30.4	-28.6
-3	9	-3	43.5	-43.5
-5	9	-3	35.3	-36.8
-4	8	-3	10.8	-9.8
2	8	-3	22.4	22.4
4	8	-3	11.5	11.9
5	7	-3	14.2	-14.5
3	7	-3	22.9	-23.6
1	7	-3	40.3	-40.6
-1	7	-3	22.2	-21.5
-2	6	-3	44.3	-44.5
0	6	-3	36.4	-38.1
2	6	-3	68.7	-69.1
4	6	-3	67.5	-65.9
6	6	-3	19.8	-20.0
5	5	-3	12.7	-12.3
3	5	-3	51.4	-52.2
1	5	-3	43.1	-44.2
-1	5	-3	17.1	-17.4
-4	4	-3	11.3	-11.4
0	4	-3	11.9	-12.7
2	4	-3	45.2	46.3
4	4	-3	22.8	22.5
7	3	-3	35.6	-35.7
5	3	-3	15.5	-14.8
3	3	-3	22.9	-22.6
1	3	-3	113.7	-113.6
-1	3	-3	88.1	-88.0
-3	3	-3	71.7	-72.1
-5	3	-3	75.5	-75.6
-7	3	-3	32.4	-32.1
-4	2	-3	21.5	-21.9
-2	2	-3	25.7	-26.8
0	2	-3	57.5	59.0
2	2	-3	15.0	15.7
4	2	-3	16.5	16.9
5	1	-3	19.4	-18.8
3	1	-3	63.5	-63.4
1	1	-3	77.4	-77.4
-1	1	-3	39.1	-40.3

H	K	L	/FO/	/FC/
-2	0	-3	57.0	-57.0
0	0	-3	121.5	-120.6
2	0	-3	52.7	-54.5
4	0	-3	89.5	-90.5
6	0	-3	40.5	-41.1
-5	3	-2	14.4	9
-3	3	-2	38.6	3
-1	3	-2	53.1	0
1	3	-2	105.7	102.2
3	3	-2	61.5	5
5	3	-2	20.7	5
7	3	-2	13.3	3
4	2	-2	20.8	3
2	2	-2	41.2	.0
0	2	-2	77.7	.2
-4	2	-2	12.0	.1
-3	1	-2	37.2	.6
-1	1	-2	83.7	.0
1	1	-2	63.2	.4
3	1	-2	17.8	.3
5	1	-2	8.6	.3
8	0	-2	26.3	.5
6	0	-2	74.0	.9
4	0	-2	103.9	101.7
2	0	-2	19.7	-18.7
-2	0	-2	114.0	114.4
-4	0	-2	29.0	28.1
-6	0	-2	32.9	33.1
-8	0	-2	34.7	34.2
6	4	-2	13.1	.1
2	4	-2	12.2	1
0	4	-2	27.1	.8
-2	4	-2	50.0	.9
-3	5	-2	28.6	.3
-1	5	-2	56.9	.7
1	5	-2	27.2	.6
3	5	-2	14.8	.8
6	6	-2	61.9	60.6
4	6	-2	51.5	.4
2	6	-2	11.8	.7
0	6	-2	21.1	.6
-2	6	-2	26.0	25.2
-4	6	-2	31.3	.3
-6	6	-2	25.6	.9
-3	7	-2	14.4	.4
-1	7	-2	31.6	1
1	7	-2	42.5	.1
2	8	-2	11.6	.3
0	8	-2	23.1	.6
-2	8	-2	22.3	.7

H	K	L	/FO/	/FC/
-5	9	-2	14.6	14.5
-3	9	-2	17.1	17.4
-1	9	-2	32.4	32.1
1	9	-2	63.3	62.0
3	9	-2	20.9	21.1
0	10	-2	18.3	18.4
-1	11	-2	14.1	-14.0
1	11	-2	19.0	-18.8
4	12	-2	19.5	21.3
-2	12	-2	11.1	10.6
-1	13	-2	12.9	-12.1
-4	12	-1	16.6	-16.5
-2	12	-1	30.4	-30.0
0	12	-1	16.8	-17.1
-3	11	-1	14.4	-14.7
-4	10	-1	13.9	13.8
-2	10	-1	14.4	14.9
5	9	-1	32.4	-32.4
3	9	-1	67.8	-66.6
1	9	-1	48.1	-47.6
-1	9	-1	13.5	-13.4
-4	8	-1	14.3	14.8
-2	8	-1	23.8	23.9
0	8	-1	12.5	11.8
2	8	-1	11.4	-11.6
3	7	-1	11.4	11.1
-3	7	-1	28.7	-29.0
-5	7	-1	16.2	-16.2
-6	6	-1	22.0	-22.0
-4	6	-1	35.0	-34.1
-2	6	-1	84.9	-85.2
0	6	-1	58.1	-59.2
2	6	-1	50.6	50.2
4	6	-1	20.6	20.1
6	6	-1	19.2	-19.9
3	5	-1	22.4	23.3
1	5	-1	16.8	16.7
-1	5	-1	37.2	-38.2
-3	5	-1	28.9	-27.7
-5	5	-1	16.2	-15.7
-6	4	-1	13.4	13.3
-4	4	-1	19.6	19.4
-2	4	-1	50.7	51.8
0	4	-1	39.3	41.4
2	4	-1	23.5	-25.4
5	3	-1	51.6	-51.8
3	3	-1	156.6	-157.3
1	3	-1	125.6	-125.9
-1	3	-1	19.6	18.3
-3	3	-1	22.7	-22.8

H	K	L	/FO/	/FC/
-5	3	-1	29.5	-29.2
-7	3	-1	14.5	-15.2
-4	2	-1	50.6	50.7
-2	2	-1	35.7	35.9
0	2	-1	9.8	11.2
2	2	-1	41.5	41.9
4	2	-1	14.4	-15.3
8	2	-1	12.2	12.3
3	1	-1	23.2	24.6
1	1	-1	13.0	12.8
-1	1	-1	39.1	-39.1
-3	1	-1	40.5	-41.9
-5	1	-1	21.9	-22.3
-6	0	-1	20.1	-20.5
-4	0	-1	72.6	-72.0
-2	0	-1	107.1	-106.8
0	0	-1	65.7	-67.5
2	0	-1	36.2	34.6
4	0	-1	52.5	52.4
6	0	-1	24.1	-23.7
8	0	-1	33.0	-31.4
7	3	0	28.1	27.6
5	3	0	67.7	68.0
3	3	0	61.4	61.6
1	3	0	35.3	-33.5
8	2	0	12.2	11.8
6	2	0	14.4	14.7
4	2	0	32.5	32.8
2	2	0	44.0	44.3
0	2	0	33.7	-32.8
5	1	0	18.6	-18.1
1	1	0	29.1	29.4
7	1	0	13.7	-13.1
6	0	0	17.0	16.7
4	0	0	13.3	12.3
2	0	0	128.6	127.7
6	4	0	25.0	24.9
4	4	0	18.6	18.8
0	4	0	42.1	43.1
5	5	0	16.7	-16.4
3	5	0	10.3	10.8
1	5	0	16.0	16.9
4	6	0	15.0	14.1
2	6	0	99.0	99.0
0	6	0	151.4	152.4
3	7	0	9.3	-8.0
1	7	0	23.9	24.8
4	8	0	13.2	12.8
6	8	0	14.8	14.3
5	9	0	32.7	32.5

H	K	L	/FO/	/FC/
3	9	0	36.3	36.8
1	9	0	19.2	-19.1
1	11	0	13.4	15.2
2	12	0	30.2	31.0
0	12	0	51.9	.8
-2	12	1	11.5	6
8	0	1	12.5	-1
6	4	2	9.8	9
-5	7	2	10.0	1
-5	9	2	14.3	-1
-1	13	3	9.1	1
-3	13	3	14.1	-1 .4
3	7	3	9.4	.8
6	6	3	11.5	.9
-7	3	4	34.5	.7
-5	3	4	35.0	.3
-3	3	4	39.3	.8
-1	3	4	56.1	.8
1	3	4	23.2	-.4
3	3	4	27.3	-.0
5	3	4	26.1	9
7	3	4	33.5	8
6	2	4	15.0	.6
4	2	4	10.1	.1
-2	2	4	20.8	-.5
-4	2	4	33.2	.6
-6	2	4	18.8	.0
-7	1	4	13.8	-.3
-5	1	4	28.8	.5
-3	1	4	33.7	.5
-1	1	4	19.1	.1
5	1	4	9.2	.1
4	0	4	87.5	.1
2	0	4	134.7	1 .0
0	0	4	66.8	.8
-2	0	4	88.2	.3
-4	0	4	26.5	.5
4	4	4	11.8	.2
2	4	4	19.5	-.1
0	4	4	21.6	-.6
-2	4	4	25.5	.4
-4	4	4	13.5	.0
-6	4	4	14.5	.6
-7	5	4	11.7	-.7
-5	5	4	17.8	-.7
-3	5	4	27.2	-.3
-1	5	4	13.4	-.3
1	5	4	19.3	.7
4	6	4	44.1	.4
2	6	4	99.5	97.6

H	K	L	/FO/	/FC/
0	6	4	69.9	70.3
-2	6	4	27.0	27.2
-4	6	4	28.0	27.9
-5	7	4	25.0	-23.9
-3	7	4	14.1	-14.0
2	8	4	9.8	-10.0
0	8	4	11.3	-10.9
-6	8	4	10.7	10.2
-5	9	4	25.6	25.4
-3	9	4	18.9	18.5
-1	9	4	13.7	13.5
3	9	4	13.8	-15.1
-5	11	4	13.7	-11.8
4	12	4	19.8	19.9
2	12	4	33.5	34.2
0	12	4	23.8	23.0
-2	12	4	14.2	12.8
-1	11	5	12.1	11.0
1	9	5	42.1	-41.8
-1	9	5	71.0	-69.3
-3	9	5	29.8	-30.2
-5	9	5	14.6	-13.9
4	8	5	16.6	17.2
3	7	5	14.9	-14.2
-1	7	5	20.1	20.8
-6	6	5	21.7	-22.2
-4	6	5	14.9	-14.5
0	6	5	25.2	25.6
2	6	5	17.0	-16.4
4	6	5	54.4	-55.3
6	6	5	22.8	-23.5
5	5	5	16.6	-17.2
3	5	5	11.5	-10.1
-3	5	5	13.9	14.1
-7	5	5	12.3	-12.3
-6	4	5	14.3	13.3
0	4	5	15.2	15.6
4	4	5	30.3	29.6
6	4	5	14.8	15.2
7	3	5	12.1	-12.4
5	3	5	15.6	15.1
1	3	5	106.6	-107.2
-1	3	5	128.6	-130.0
-3	3	5	71.5	-72.4
-5	3	5	32.0	-31.5
-7	3	5	11.9	-13.0
-4	2	5	13.7	13.9
-2	2	5	12.7	-14.0
0	2	5	9.4	-9.7
2	2	5	45.2	45.1

Table 8. Observed (FO) and calculated (FC) structure factors for sample 6. Tae23-1a.

H	K	L	/FO/	/FC/
-4	12	-1	13.2	-13.6
-2	12	-1	28.9	-28.4
0	12	-1	14.8	-14.5
2	12	-1	16.6	17.3
-3	11	-1	14.3	-14.1
-4	10	-1	14.7	13.9
-2	10	-1	16.1	15.0
5	9	-1	29.3	-29.1
3	9	-1	62.6	-62.7
1	9	-1	43.2	-41.2
-4	8	-1	17.3	17.1
-2	8	-1	27.3	26.2
0	8	-1	14.1	13.4
2	8	-1	9.9	-9.6
5	7	-1	10.9	10.7
3	7	-1	10.5	10.2
-3	7	-1	29.2	-29.7
-5	7	-1	15.7	-16.1
-6	6	-1	16.0	-16.2
-4	6	-1	27.0	-26.9
-2	6	-1	76.6	-76.6
0	6	-1	49.9	-50.0
2	6	-1	59.4	58.5
4	6	-1	27.3	27.6
6	6	-1	16.1	-16.0
3	5	-1	24.3	24.7
1	5	-1	18.7	19.0
-1	5	-1	36.6	-37.0
-3	5	-1	24.9	-25.7
-5	5	-1	14.2	-13.7
-6	4	-1	11.9	12.0
-4	4	-1	19.4	19.5
-2	4	-1	52.5	53.2
0	4	-1	40.5	40.4
2	4	-1	24.7	-25.9
5	3	-1	44.7	-44.3
3	3	-1	145.6	-145.2
1	3	-1	110.9	-111.7
-1	3	-1	38.0	37.7
-3	3	-1	10.6	-11.5
-5	3	-1	21.7	-22.9
-4	2	-1	50.8	51.6
-2	2	-1	35.0	36.9
0	2	-1	10.1	9.3
2	2	-1	41.5	42.1
4	2	-1	13.8	-14.6
6	2	-1	13.2	12.7
3	1	-1	23.0	23.4
1	1	-1	13.1	13.1
-1	1	-1	38.6	-39.3
-3	1	-1	38.8	40.7
-5	1	-1	20.3	20.5
-6	0	-1	13.0	13.7
-4	0	-1	60.1	60.4
-2	0	-1	90.1	91.4
0	0	-1	55.4	53.7
2	0	-1	49.2	49.0
4	0	-1	59.2	59.6
6	0	-1	18.2	17.4
8	0	-1	27.0	28.2
7	1	0	12.7	12.6
5	1	0	17.1	18.1
1	1	0	29.9	30.0
6	0	0	11.2	10.7
2	0	0	110.6	107.0
8	2	0	11.9	11.5
6	2	0	14.7	15.2
4	2	0	32.7	33.6
2	2	0	40.8	41.3
0	2	0	36.7	-37.9
7	3	0	23.4	23.6
5	3	0	63.5	62.0
3	3	0	49.2	51.2
1	3	0	49.9	-50.2
6	4	0	27.5	26.2
4	4	0	19.0	19.6
0	4	0	42.7	42.9
7	5	0	11.6	-11.6
5	5	0	17.9	-16.7
3	5	0	11.4	11.2
1	5	0	13.4	14.0
2	6	0	89.5	89.2
0	6	0	144.0	141.9
1	7	0	27.1	28.2
4	8	0	12.5	12.1
6	8	0	14.1	14.3
5	9	0	29.4	30.3
3	9	0	33.2	32.8
1	9	0	26.7	-26.3
4	10	0	10.5	10.0
1	11	0	13.3	13.0
2	12	0	28.9	29.1
0	12	0	50.4	51.5
7	3	1	11.6	-10.8
-3	1	2	18.1	-19.2
-1	1	2	62.8	-61.6
1	1	2	83.3	-81.4
3	1	2	35.3	-34.5
8	0	2	29.9	30.7
6	0	2	28.2	27.3
4	0	2	22.4	22.2
2	0	2	105.1	103.6
0	0	2	15.0	-13.6
-2	0	2	37.3	-38.4
-4	0	2	89.7	91.2
-6	0	2	69.0	67.5
-8	0	2	20.6	20.8
4	2	2	10.0	10.1
0	2	2	82.3	81.5
-2	2	2	38.5	40.3
-4	2	2	21.2	-22.7
-7	3	2	20.1	-19.4
-5	3	2	30.1	-28.2
-3	3	2	49.4	51.2
-1	3	2	90.7	91.1
1	3	2	37.3	39.2
3	3	2	27.4	28.6
6	4	2	10.1	-9.9
2	4	2	48.7	50.5
0	4	2	29.2	29.5
-2	4	2	12.2	12.5
-6	4	2	14.9	-13.4
-3	5	2	17.3	-17.4
-1	5	2	28.2	-29.4
1	5	2	59.6	-60.8
3	5	2	28.9	-30.4
6	6	2	21.6	22.4
4	6	2	23.8	24.9
2	6	2	17.9	18.7
0	6	2	11.2	11.5
-4	6	2	44.0	42.8
-6	6	2	57.7	56.2
-5	7	2	9.7	9.7
-1	7	2	43.7	-44.4
1	7	2	31.6	-31.0
3	7	2	11.9	-11.9
2	8	2	20.3	21.1
0	8	2	22.9	21.6
-5	9	2	18.5	-18.2
-3	9	2	17.3	16.3
-1	9	2	60.2	58.5
1	9	2	26.8	26.1
3	9	2	11.1	11.3
2	10	2	10.6	11.5
0	10	2	20.3	18.9
-1	11	2	22.1	-21.0
1	11	2	16.1	-16.4
-4	12	2	18.4	18.3
1	13	2	12.0	-12.7
-3	13	3	13.8	-13.9
-4	12	3	26.5	-25.6
-2	12	3	22.5	-21.6
0	12	3	16.7	-15.5
-1	11	3	18.8	-18.5
-3	11	3	12.4	-11.2
-2	10	3	11.6	12.1
5	9	3	35.6	-35.0
3	9	3	39.9	-41.3
1	9	3	24.8	-24.3
-1	9	3	22.2	-21.6
-3	9	3	11.3	-10.3
-4	8	3	14.7	13.4
-2	8	3	25.5	24.1
1	7	3	23.2	-23.2
-1	7	3	41.7	-42.0
-3	7	3	23.4	-23.5
-5	7	3	17.4	-15.7
-4	6	3	61.8	-61.2
-2	6	3	60.4	-60.1
0	6	3	27.4	-28.3
2	6	3	34.6	-36.2
6	6	3	13.7	14.5
1	5	3	14.2	-14.2
-1	5	3	41.6	-42.6
-3	5	3	52.2	-52.8
-5	5	3	12.2	-11.8
-4	4	3	22.4	22.1
-2	4	3	44.2	44.7
0	4	3	14.6	-14.4
4	4	3	11.2	-11.4
7	3	3	27.7	-28.5
5	3	3	68.3	-70.1
3	3	3	61.8	-63.9
1	3	3	79.4	-79.6
-1	3	3	100.6	-102.3
-3	3	3	11.2	-12.1
-7	3	3	32.0	-31.3
-4	2	3	15.3	16.4
-2	2	3	17.0	17.7
0	2	3	62.5	61.2
2	2	3	25.1	-26.4
4	2	3	22.1	-22.8
1	1	3	38.8	-37.8
-1	1	3	75.9	-77.1
-3	1	3	61.1	-63.1
-5	1	3	19.0	-19.3
-8	0	3	14.5	14.7
-6	0	3	36.0	-35.3
-4	0	3	79.7	-79.6
-2	0	3	37.6	-39.1
0	0	3	104.5	-103.2
2	0	3	43.9	-44.1
4	0	3	15.7	16.9
-7	1	4	13.5	-14.2
-5	1	4	28.8	-29.3
-3	1	4	33.0	-31.8
-1	1	4	18.3	-17.3
1	1	4	7.6	8.7
5	1	4	10.7	-10.6
4	0	4	77.8	80.4
2	0	4	117.1	118.3
0	0	4	55.9	54.0
-2	0	4	80.8	81.1
-4	0	4	19.3	19.0
6	2	4	13.4	14.3
4	2	4	9.6	-9.6
-2	2	4	23.2	-23.8
-4	2	4	32.3	33.3
-6	2	4	21.8	20.8
-7	3	4	33.2	32.3
-5	3	4	28.6	28.4
-3	3	4	27.4	28.8
-1	3	4	43.8	45.0
1	3	4	38.4	-37.2
3	3	4	33.1	-33.1
5	3	4	19.9	20.9
7	3	4	30.4	31.3
4	4	4	11.6	11.6
2	4	4	19.2	-19.2
0	4	4	23.0	-22.1
-2	4	4	26.1	26.3
-4	4	4	14.7	14.0
-6	4	4	14.4	14.6
-5	5	4	19.1	-19.4
-3	5	4	27.8	-27.6
-1	5	4	15.1	-14.8
1	5	4	19.3	18.8
5	5	4	10.9	-11.5
4	6	4	38.5	38.3
2	6	4	89.1	91.1
0	6	4	64.1	64.1
-2	6	4	22.2	21.1
-4	6	4	24.7	22.3
-5	7	4	25.5	-24.2
-3	7	4	14.4	-13.2
2	8	4	10.9	-11.6
0	8	4	14.2	-13.8
-4	8	4	10.5	9.9
-6	8	4	11.0	10.3
-5	9	4	24.9	22.7
-3	9	4	13.4	13.2
3	9	4	19.3	-20.4
-4	10	4	11.2	10.9
-5	11	4	15.6	-14.2
4	12	4	16.9	17.5
2	12	4	31.5	33.3
0	12	4	20.4	21.0
-2	12	4	10.4	9.6
0	12	5	12.9	13.9
-1	11	5	14.4	13.6
3	9	5	10.6	10.6
1	9	5	37.1	-37.1
-1	9	5	68.4	-67.6
-3	9	5	27.0	-26.5
4	8	5	18.6	19.2
3	7	5	16.0	-16.9
-1	7	5	23.7	22.3
-6	6	5	17.8	-17.0
-2	6	5	16.7	16.9
0	6	5	34.1	33.8
2	6	5	11.6	-12.3
4	6	5	50.9	-52.7
6	6	5	18.1	-20.5
5	5	5	16.9	-18.1
3	5	5	9.6	-9.9
-3	5	5	17.6	17.8
-7	5	5	11.8	-12.2
-6	4	5	13.0	13.9
-4	4	5	12.0	-11.3
0	4	5	17.8	17.5
4	4	5	31.2	30.5
6	4	5	15.2	15.9
5	3	5	20.5	20.9
1	3	5	98.8	-96.4
-1	3	5	119.6	-119.0
-3	3	5	64.5	-65.2
-5	3	5	26.9	-25.7
-4	2	5	15.4	15.2
-2	2	5	11.7	-12.5
2	2	5	48.4	48.2
4	2	5	25.3	25.0
6	2	5	13.0	13.9
5	1	5	19.6	-19.3
3	1	5	18.3	-18.2
-1	1	5	9.9	9.7
-3	1	5	13.1	14.3
-7	1	5	12.7	-12.8
-8	0	5	14.4	-15.7
-6	0	5	13.7	-13.0
-4	0	5	36.4	-37.2

Table 8. Observed (FO) and calculated (FC) structure factors for sample 7. Tae23-1b.

H	K	L	/FO/	/FC/
1	13	0	7.5	8.0
2	12	0	31.4	32.6
0	12	0	61.4	59.0
1	11	0	15.4	14.9
6	10	0	10.4	11.1
4	10	0	9.5	10.1
0	10	0	5.9	-6.5
5	9	0	34.3	34.7
3	9	0	35.8	36.6
1	9	0	26.7	-27.4
6	8	0	15.9	16.0
4	8	0	13.7	13.5
7	7	0	6.6	-7.4
5	7	0	7.9	-8.3
3	7	0	8.4	-8.1
1	7	0	26.7	28.4
4	6	0	7.5	8.0
2	6	0	92.6	93.4
0	6	0	147.0	148.9
7	5	0	13.0	-12.9
5	5	0	17.9	-18.0
3	5	0	11.1	11.9
1	5	0	14.3	15.3
8	4	0	6.5	7.0
6	4	0	28.2	27.5
4	4	0	18.9	19.2
0	4	0	41.0	41.6
7	3	0	27.5	27.1
5	3	0	66.4	66.1
3	3	0	52.1	53.3
1	3	0	47.6	-47.5
8	2	0	12.3	12.4
6	2	0	15.2	15.6
4	2	0	32.8	34.2
2	2	0	39.8	40.8
0	2	0	35.5	-37.0
7	1	0	13.8	-13.8
5	1	0	18.3	-18.9
3	1	0	5.2	5.6
1	1	0	30.1	30.8
6	0	0	12.7	12.1
2	0	0	113.2	115.4
2	14	1	9.5	9.5
-3	13	1	8.6	8.7
1	13	1	9.6	-9.2
3	13	1	7.8	-8.2
4	12	1	16.9	-16.9
2	12	1	34.4	-33.7
0	12	1	18.5	-17.7
-2	12	1	19.3	18.6
-4	12	1	14.1	14.5
-5	11	1	7.7	8.4
-3	11	1	9.3	8.9
3	11	1	16.8	-16.1
5	11	1	8.6	-9.0
4	10	1	15.5	15.6
2	10	1	17.6	17.1
-5	9	1	33.0	-33.7
-3	9	1	68.3	-69.0		9	1	45.9	-45.0		9	1	8.1	-7.7		9	1	5.1	5.0		9	1	8.7	-9.0		8	1	8.4	8.3		8	1	17.8	17.9		8	1	27.1	27.1		8	1	13.2	13.2		8	1	10.5	-10.9		7	1	5.3	-5.6		7	1	12.2	12.2		7	1	10.8	11.3		7	1	30.4	-30.8		7	1	17.7	-17.7		6	1	19.7	-19.3		6	1	30.0	-30.1		6	1	80.4	-81.1		6	1	51.5	-52.7		6	1	59.1	59.3		6	1	27.1	27.7		5	1	25.1	25.7		5	1	18.5	19.4		5	1	36.4	-38.0		5	1	26.4	-26.8		5	1	14.0	-14.0		4	1	13.9	13.4		4	1	20.1	20.2		4	1	52.5	53.7		4	1	39.3	40.2		4	1	25.7	-26.4		3	1	47.5	-47.1		3	1	149.8	-150.6		3	1	115.1	-114.3		3	1	36.3	35.8		3	1	11.7	-12.0		3	1	25.0	-24.6		3	1	12.2	-12.6		2	1	6.1	6.2		2	1	51.2	52.8		2	1	34.4	36.7		2	1	11.2	10.3		-2	2	1	40.2	41.2
-4	2	1	14.4	-15.7
-8	2	1	13.6	14.2
-5	1	1	6.0	6.5
-3	1	1	23.2	24.7
-1	1	1	13.1	14.3
1	1	1	37.7	-38.2
3	1	1	38.8	-40.7
5	1	1	20.7	-21.0
6	0	1	15.9	-16.2
4	0	1	62.4	-64.1
2	0	1	92.0	-93.4
0	0	1	54.9	-52.1
-2	0	1	47.3	47.1
-4	0	1	58.9	60.0
-6	0	1	17.7	-19.6
-8	0	1	30.6	-32.3
0	14	2	7.6	7.6
3	13	2	7.1	-7.1
1	13	2	15.1	-14.7
2	12	2	8.4	8.7
4	12	2	7.8	8.4
3	11	2	7.2	-7.1
1	11	2	17.5	-17.1
-1	11	2	23.9	-23.1
-2	10	2	9.3	9.1
0	10	2	20.3	20.2
2	10	2	12.5	12.7
5	9	2	13.2	13.4
3	9	2	13.7	13.7
1	9	2	29.3	29.2
-1	9	2	64.7	63.5
-3	9	2	18.2	18.8
-5	9	2	18.4	-18.8
-6	8	2	10.2	-10.3
-2	8	2	9.7	9.9
0	8	2	22.8	22.7
2	8	2	21.9	21.9
6	8	2	6.8	-7.1
3	7	2	13.3	-12.8
1	7	2	31.2	-32.3
-1	7	2	45.4	-45.0
-5	7	2	10.7	10.5
-6	6	2	61.8	61.4
-4	6	2	45.5	45.6
0	6	2	11.5	11.9
2	6	2	19.9	19.6
4	6	2	27.0	26.8
6	6	2	24.9	25.4
5	5	2	4.8	4.8

H	K	L	/FO/	/FC/
3	5	2	30.0	-30.2
1	5	2	58.9	-60.4
-1	5	2	27.3	-28.6
-3	5	2	16.6	-17.1
-5	5	2	4.9	5.3
-7	5	2	9.4	9.5
-6	4	2	14.8	-14.6
-4	4	2	7.0	6.9
-2	4	2	11.3	12.0
0	4	2	27.0	28.7
2	4	2	49.8	50.6
4	4	2	4.7	-4.5
6	4	2	10.9	-10.8
5	3	2	8.9	9.4
3	3	2	29.0	31.0
1	3	2	40.6	41.8
-1	3	2	92.2	92.4
-3	3	2	52.2	53.1
-5	3	2	27.7	-27.5
-6	2	2	5.5	-5.8
-4	2	2	22.1	-23.3
-2	2	2	38.3	39.4
0	2	2	78.1	79.5
4	2	2	10.0	9.8
6	2	2	7.1	-7.0
8	2	2	9.8	-9.9
3	1	2	34.6	-35.7
1	1	2	81.9	-83.8
-1	1	2	62.5	-63.2
-3	1	2	18.3	-19.0
-5	1	2	8.2	8.3
-7	1	2	8.5	8.1
-8	0	2	72.1	71.2
-4	0	2	91.8	93.6
-2	0	2	36.3	-35.7
0	0	2	15.6	-13.5
2	0	2	100.4	102.5
4	0	2	22.6	22.9
6	0	2	30.3	29.7
8	0	2	34.2	35.0
-7	3	2	17.4	-19.3
-4	12	2	20.9	21.8
-1	13	2	6.8	-6.7
-2	14	3	7.2	7.7
-3	13	3	15.5	-15.6
-1	13	3	11.3	-11.1
2	12	3	13.5	-12.7
0	12	3	18.9	-18.0
-2	12	3	25.2	-24.8
-4	12	3	28.9	-29.8
1	11	3	7.4	-8.7
1	11	3	11.9	-12.0
1	11	3	20.5	-19.7
1	11	3	9.5	-9.1
1	11	3	7.7	7.9
0	10	3	9.2	-9.2
0	10	3	9.1	-8.3
0	10	3	6.8	6.7
0	10	3	13.4	13.4
0	10	3	8.4	9.1
9	3	3	11.7	-11.5
9	3	3	24.0	-23.2
9	3	3	26.5	-25.5
9	3	3	45.2	-44.4
9	3	3	38.2	-39.0
8	3	3	6.7	-6.3
8	3	3	10.7	-10.6
8	3	3	4.4	4.1
8	3	3	23.9	24.0
8	3	3	12.9	13.2
7	3	3	16.1	-16.3
7	3	3	24.0	-23.8
7	3	3	41.6	-42.1
7	3	3	22.8	-23.1
7	3	3	10.5	10.6
6	3	3	14.9	14.6
6	3	3	4.8	4.9
6	3	3	37.3	-38.1
6	3	3	28.8	-30.1
6	3	3	61.2	-61.8
6	3	3	63.3	-64.0
6	3	3	18.5	-18.6
5	3	3	11.4	-11.7
5	3	3	52.7	-52.6
5	3	3	41.0	-42.1
5	3	3	14.0	-13.7
5	3	3	7.4	-7.4
5	3	3	6.9	6.7
4	3	3	12.0	-11.6
4	3	3	11.8	-11.6
4	3	3	13.5	-13.8
4	3	3	43.8	44.4
4	3	3	22.2	22.5
4	3	3	6.5	-6.6
3	3	3	34.3	-33.9
3	3	3	8.5	-8.0
3	3	3	12.0	-12.5
3	3	3	100.2	-100.9
3	3	3	79.3	-79.0
3	3	3	63.7	-64.0
5	3	3	74.9	-72.9
7	3	3	30.9	-31.3
4	2	3	22.7	-23.2
2	2	3	24.8	-26.3
0	2	3	58.7	57.9
-2	2	3	14.9	16.1
-4	2	3	15.3	15.8
-6	2	3	8.4	7.7
-8	2	3	10.6	-10.0
-5	1	3	19.1	-19.0
-3	1	3	60.0	-61.8
-1	1	3	74.9	-75.1
1	1	3	37.7	-36.5
3	1	3	5.4	-5.3
5	1	3	4.7	4.9
8	0	3	9.0	-10.1
6	0	3	7.0	7.5
4	0	3	14.6	15.2
2	0	3	43.7	-45.7
0	0	3	107.7	-104.7
-2	0	3	40.9	-41.2
-4	0	3	80.7	-80.9
-6	0	3	38.0	-37.5
0	14	4	5.9	-5.6
1	13	4	9.4	8.9
-3	13	4	5.8	-6.1
-2	12	4	10.8	11.1
0	12	4	24.5	23.4
2	12	4	39.4	37.4
4	12	4	20.3	20.5
-3	11	4	7.4	-7.3
-5	11	4	13.3	-14.8
-4	10	4	10.7	11.3
0	10	4	7.4	-7.2
2	10	4	7.9	-7.7
5	9	4	10.2	10.3
3	9	4	21.9	-20.3
-1	9	4	8.4	8.6
-3	9	4	14.9	15.0
-5	9	4	24.4	25.1
-6	8	4	10.0	10.6
-4	8	4	9.5	10.4
-2	8	4	6.2	6.0
0	8	4	13.8	-13.3
2	8	4	11.8	-11.5
3	7	4	7.3	6.8
-1	7	4	6.3	6.3
-3	7	4	12.8	-13.0
-5	7	4	25.0	-24.9
-7	7	4	6.6	-7.3

Sample 7. Tae23-1b (continued)

H	K	L	/FO/	/FC/
4	4	9	8.3	8.4
0	4	9	20.1	-20.4
-6	4	9	5.2	5.3
-7	3	9	6.9	7.1
-5	3	9	22.4	-22.2
-3	3	9	50.6	-50.8
-1	3	9	54.7	-55.3
1	3	9	50.6	-49.6
3	3	9	27.1	-27.8
6	2	9	8.8	9.4
-2	2	9	21.1	-21.1
-6	2	9	14.9	15.1
-7	1	9	11.4	-12.1
-5	1	9	12.5	-13.3
-3	1	9	5.0	-5.1
3	1	9	12.5	-12.7
5	1	9	10.5	-10.8
6	0	9	26.7	-27.0
4	0	9	11.1	-11.0
0	0	9	18.1	-20.3
-2	0	9	11.1	12.1
-6	0	9	34.1	-33.4
3	9	10	19.3	19.9
1	9	10	11.7	11.9
-4	8	10	7.6	-8.0
4	8	10	7.4	7.6
3	7	10	7.7	-8.3
1	7	10	12.9	-13.4
-3	7	10	5.1	5.0
-6	6	10	19.8	21.0
-4	6	10	27.3	27.3
-2	6	10	24.0	23.7
0	6	10	26.7	26.6
4	6	10	10.3	-10.1
3	5	10	11.6	-12.1
1	5	10	7.8	-7.7
-5	5	10	7.0	6.9
-4	4	10	11.8	-12.4
0	4	10	5.3	5.9
2	4	10	9.0	9.2
4	4	10	12.4	13.2
5	3	10	20.1	20.7
3	3	10	31.3	32.8
1	3	10	9.0	10.0
-5	3	10	8.3	-8.2
-2	2	10	10.8	-11.9
0	2	10	10.6	11.2
2	2	10	16.4	18.5
5	1	10	7.6	-7.4
3	1	10	13.1	-14.0
1	1	10	12.7	-13
-1	1	10	7.4	-7
-5	1	10	5.7	5
-6	0	10	23.7	26
-4	0	10	25.0	27
-2	0	10	45.1	47
0	0	10	31.7	32
4	0	10	4.7	-4
2	10	10	6.2	6
0	10	11	7.8	8
2	8	11	6.7	6.
-2	8	11	8.5	8.
1	7	11	8.9	-8
2	6	11	17.5	-17
0	6	11	31.1	-31.
-2	6	11	10.4	-9.
-1	5	11	13.7	-13
2	4	11	6.7	7
0	4	11	19.3	20.
-2	4	11	13.4	13.
-7	3	11	13.0	-13.
-5	3	11	20.5	-21.
-3	3	11	25.2	-25.
3	3	11	9.3	-9.
5	3	11	20.3	-20.
2	2	11	18.0	19.
0	2	11	12.0	13.
-4	2	11	8.9	9.
-3	1	11	5.8	-5.
-1	1	11	12.5	-13.
1	1	11	11.1	-12.
2	0	11	29.5	-31.
0	0	11	28.6	-31.
-2	0	11	8.4	-9.
-2	10	12	8.1	7.
-1	9	12	18.3	18.
-3	9	12	23.5	23.
-4	8	12	6.8	7.
-2	8	12	8.4	8.
0	8	12	7.8	7.
-3	7	12	9.3	-9.
2	6	12	29.5	29.
3	5	12	8.1	7.
-1	5	12	7.2	-7.
-5	5	12	6.0	-5.
-6	4	12	7.0	6.
-4	4	12	10.2	10.
-2	4	12	10.1	10.
0	4	12	13.1	13.
3	3	12	11.7	-12.
-1	3	12	28.4	30.0
-3	3	12	28.0	30.2
-5	3	12	10.6	11.1
-4	2	12	12.2	12.5
-2	2	12	17.9	20.5
3	1	12	7.1	7.2
-1	1	12	7.8	-8.5
-3	1	12	7.8	-8.9
-6	0	12	18.6	19.4
-2	0	12	10.5	-11.8
0	0	12	19.7	22.9
2	0	12	32.9	36.0
4	0	12	20.5	20.6
-1	9	13	18.7	-17.9
1	7	13	7.0	6.5
0	6	13	11.3	11.5
-2	6	13	6.3	6.1
-4	6	13	18.2	-17.8
-5	5	13	7.1	-7.5
-4	4	13	9.6	9.9
-5	3	13	9.4	8.9
-3	3	13	8.2	-8.9
-1	3	13	31.5	-34.2
1	3	13	22.4	-23.8
3	3	13	7.2	-7.2
-2	2	13	6.7	7.1
-6	2	13	6.3	6.5
1	1	13	5.1	4.7
4	0	13	12.2	-11.4
0	0	13	16.6	17.1
-4	0	13	15.1	-16.1
-6	0	13	17.4	-18.0
-4	6	14	18.0	17.4
-2	6	14	19.0	18.2
1	5	14	5.5	-5.1
-2	4	14	6.7	-5.8
1	3	14	8.3	8.1
-3	3	14	11.2	-11.1
-4	2	14	5.9	-5.9
3	1	14	8.5	-7.8
1	1	14	5.9	-6.0
-4	0	14	27.1	27.3
-2	0	14	22.7	22.6
2	0	14	6.1	5.4
-2	6	15	11.0	-10.1
-1	5	15	7.4	-6.4
1	3	15	6.6	-6.6
0	2	15	9.0	8.2
-1	1	15	8.3	-7.9
1	1	15	8.4	-7.2
2	0	15	10.6	-8.9
0	0	15	14.1	-12.8
-2	0	15	8.8	-7.7
-1	3	16	10.0	8.
-1	1	16	6.1	-5.
-3	1	16	6.9	-5.7
-2	0	16	6.3	5.5

Table 8. Observed (FO) and calculated (FC) structure factors for sample 8. Tae23-1c.

H	K	L	/FO/	/FC/
0	12	0	44.6	43.8
1	11	0	11.2	10.9
4	10	0	8.2	7.6
6	10	0	7.1	6.2
5	9	0	23.6	21.6
3	9	0	26.2	27.1
1	9	0	20.8	-22.4
6	8	0	9.5	9.1
4	8	0	10.7	9.6
3	7	0	6.9	-6.7
1	7	0	23.5	25.0
4	6	0	6.6	7.7
2	6	0	83.6	84.2
0	6	0	136.9	141.0
5	5	0	13.6	-13.6
3	5	0	9.8	9.9
1	5	0	12.5	13.1
6	4	0	20.0	18.0
4	4	0	16.0	15.5
0	4	0	44.7	43.0
7	3	0	16.4	16.0
5	3	0	50.4	48.9
3	3	0	46.8	48.7
1	3	0	46.7	-44.5
6	2	0	11.0	9.9
4	2	0	27.0	27.3
2	2	0	40.0	39.7
0	2	0	35.0	-36.7
7	1	0	8.8	-8.1
5	1	0	14.6	-14.5
3	1	0	4.5	5.6
1	1	0	26.8	28.7
6	0	0	8.5	9.0
2	0	0	108.5	109.9
4	12	1	12.5	-12.1
2	12	1	23.0	-23.5
3	11	1	11.6	-11.4
4	10	1	11.7	10.8
2	10	1	13.6	13.6
-3	9	1	53.7	-53.5
-1	9	1	38.9	-39.9
1	9	1	8.0	-8.5
4	8	1	14.6	13.6
2	8	1	23.0	23.4
0	8	1	12.0	11.9
-2	8	1	8.3	-8.7
-3	7	1	9.2	8.6
-3	7	1	26.2	-26.4
5	7	1	13.0	-12.3
6	6	1	13.2	-13.0

H	K	L	/FO/	/FC/
4	0	1	24.1	-24.5
2	0	1	72.6	-72.6
0	0	1	47.0	-49.3
-2	0	1	51.3	52.3
-4	0	1	18.2	20.1
-3	0	1	21.6	20.9
-1	0	1	16.6	18.1
1	0	1	34.7	-34.8
3	0	1	22.3	-22.8
5	0	1	10.6	-10.4
6	0	1	9.5	8.9
4	0	1	17.0	16.7
2	0	1	49.9	48.8
0	0	1	35.7	37.4
-2	0	1	25.5	-24.7
-5	0	1	34.4	-35.7
-3	0	1	133.2	-136.8
-1	0	1	113.7	-114.3
1	0	1	34.5	33.0
3	0	1	12.0	-13.2
5	0	1	20.1	-18.0
7	0	1	7.4	-7.4
4	0	1	44.4	44.7
2	0	1	34.5	33.8
-2	0	1	40.4	40.5
-4	0	1	11.6	-13.1
-3	0	1	19.6	20.0
-1	0	1	13.9	12.6
1	0	1	35.4	-37.5
3	0	1	36.7	-37.2
5	0	1	16.9	-16.5
6	0	1	11.1	-11.6
4	0	1	55.1	-54.0
2	0	1	88.7	-90.2
0	0	1	58.6	-52.6
-2	0	1	41.3	42.6
-4	0	1	48.2	49.1
-6	0	1	17.0	-15.8
-5	0	1	23.7	-22.4
1	0	1	10.6	-10.4
-4	0	1	16.0	14.7
1	0	2	14.2	-13.9
-1	0	2	18.8	-18.6
-2	0	2	7.6	7.9
0	0	2	17.9	17.9
2	0	2	10.7	11.0
3	0	2	13.0	12.2
-1	0	2	25.8	26.7
-3	0	2	53.6	53.3
-5	0	2	15.0	13.2

H	K	L	/FO/	/FC/
-2	8	2	8.1	8.4
0	8	2	19.9	20.1
2	8	2	19.3	18.9
3	7	2	11.4	-11.0
1	7	2	28.7	-29.8
1	7	2	40.3	-40.8
-6	6	2	37.7	38.3
-4	6	2	37.5	37.4
0	6	2	10.7	12.4
2	6	2	17.1	17.9
4	6	2	22.3	21.4
6	6	2	16.4	17.4
3	5	2	25.9	-26.4
1	5	2	59.0	-58.7
-1	5	2	27.3	-27.1
-3	5	2	15.4	-15.0
-4	4	2	5.6	5.9
-2	4	2	12.3	11.0
0	4	2	28.5	28.9
2	4	2	48.1	49.4
3	3	2	28.3	29.2
1	3	2	42.3	41.3
-1	3	2	91.6	90.9
-3	3	2	45.5	47.6
-5	3	2	18.5	-20.3
-4	2	2	18.0	-19.6
-2	2	2	35.5	36.3
0	2	2	81.3	80.0
1	2	2	9.0	9.0
1	1	2	32.1	-32.5
1	1	2	86.2	-83.5
-1	1	2	59.5	-61.0
-3	1	2	16.2	-16.1
-6	0	2	45.8	47.5
-4	0	2	81.2	81.4
-2	0	2	34.3	-32.4
0	0	2	11.0	-10.2
2	0	2	102.0	101.6
4	0	2	20.6	18.9
6	0	2	22.1	21.4
5	0	2	19.4	17.6
-3	13	3	11.3	-10.5
-1	13	3	8.1	-8.4
0	12	3	14.4	-14.6
-2	12	3	19.8	-19.8
-4	12	3	19.8	-18.4
-3	11	3	8.7	-8.6
-1	11	3	15.4	-15.2
1	11	3	6.7	-7.2
4	10	3	7.2	-6.7

H	K	L	/FO/	/FC/
2	10	3	6.0	-6.3
0	10	3	6.5	6.1
-2	10	3	12.1	11.1
-4	10	3	6.7	6.7
-3	9	3	8.5	-8.5
-1	9	3	18.7	-18.5
1	9	3	21.8	-22.6
3	9	3	35.1	-36.0
5	9	3	26.4	-25.3
4	8	3	8.2	-7.1
0	8	3	4.6	5.1
-2	8	3	20.4	21.5
-4	8	3	10.9	10.6
-5	7	3	10.9	-11.8
-3	7	3	20.4	-20.7
-1	7	3	39.6	-39.8
1	7	3	21.2	-20.8
3	7	3	9.3	9.1
6	6	3	10.2	8.8
2	6	3	32.6	-33.8
0	6	3	29.8	-29.7
-2	6	3	57.7	-57.4
-4	6	3	49.3	-50.2
-5	5	3	9.0	-8.4
-3	5	3	45.7	-45.9
-1	5	3	40.7	-41.1
1	5	3	13.5	-13.4
3	5	3	6.3	-5.6
6	4	3	7.5	-7.4
4	4	3	10.1	-9.7
0	4	3	13.3	-12.6
-2	4	3	41.7	43.1
-4	4	3	18.5	18.1
-3	3	3	10.8	-11.8
-1	3	3	99.9	-100.8
1	3	3	78.2	-76.4
3	3	3	58.2	-57.8
5	3	3	56.8	-55.3
7	3	3	19.2	-17.2
4	2	3	19.3	-18.9
2	2	3	25.7	-25.8
0	2	3	61.1	59.7
-2	2	3	15.9	16.0
-4	2	3	13.6	13.6
-5	1	3	14.8	-14.3
-3	1	3	56.1	-57.3
-1	1	3	78.1	-76.6
1	1	3	38.5	-36.7
4	0	3	12.9	13.3
2	0	3	44.2	-46.3

H	K	L	/FO/	/FC/
0	0	3	112.0	-108.8
-2	0	3	40.7	-39.7
-4	0	3	69.5	-69.5
-6	0	3	23.2	-24.7
-6	0	3	11.1	-10.5
1	0	4	6.1	6.8
-2	0	4	9.5	9.2
0	0	4	20.6	20.4
2	0	4	27.9	27.3
4	0	4	14.2	12.4
-5	0	4	9.1	-9.0
0	0	4	6.2	-6.1
2	0	4	5.4	-5.9
5	0	4	8.3	7.3
3	0	4	15.2	-15.2
-1	0	4	6.2	6.3
-3	0	4	12.8	13.0
-5	0	4	18.0	18.4
-6	0	4	6.9	6.6
-4	0	4	9.2	7.9
0	0	4	11.4	-11.3
1	0	4	10.3	-10.4
-1	0	4	6.0	6.5
-3	0	4	11.4	-11.1
-5	0	4	16.3	-17.4
-4	0	4	18.9	18.5
-2	0	4	21.1	20.8
0	0	4	61.2	60.4
2	0	4	85.8	84.9
4	0	4	31.5	31.4
5	0	4	7.6	-7.5
1	0	4	18.2	18.3
-1	0	4	14.1	-12.9
-3	0	4	23.9	-23.8
-5	0	4	14.2	-13.7
-7	0	4	8.8	-8.0
-6	0	4	10.3	10.4
-4	0	4	12.0	12.1
-2	0	4	23.6	24.2
0	0	4	21.2	-21.8
2	0	4	17.9	-17.9
4	0	4	8.6	9.5
7	0	4	19.4	19.1
5	0	4	17.1	17.3
3	0	4	29.5	-29.5
1	0	4	35.6	-33.6
-1	0	4	44.3	46.3
-3	0	4	28.1	28.6
-5	0	4	24.1	24.0
-7	0	4	21.3	20.2

H	K	L	/FO/	/FC/
-6	2	4	13.7	13.4
-4	2	4	29.0	29.9
-2	2	4	22.2	-21.8
4	2	4	8.2	-8.2
6	2	4	9.6	9.9
5	1	4	7.8	-8.0
1	1	4	8.4	8.6
-1	1	4	15.4	-14.6
-3	1	4	30.1	-29.9
-5	1	4	21.3	-21.9
-7	1	4	9.5	-8.5
-4	0	4	17.7	17.4
-2	0	4	79.5	77.5
0	0	4	56.6	54.1
2	0	4	117.6	116.0
4	0	4	66.8	65.9
-4	10	4	9.5	8.7
2	12	5	8.3	-7.7
0	12	5	10.9	9.9
-1	11	5	10.8	11.2
4	10	5	7.5	8.4
2	10	5	7.5	7.5
-5	9	5	8.4	-8.5
-3	9	5	22.9	-23.6
-1	9	5	59.4	-59.4
1	9	5	33.6	-32.9
3	9	5	7.0	6.9
6	8	5	6.9	6.3
4	8	5	14.1	14.4
2	8	5	7.7	7.7
-1	7	5	20.8	19.8
3	7	5	14.0	-14.2
6	6	5	14.4	-14.3
4	6	5	42.8	-42.4
2	6	5	13.5	-12.8
0	6	5	30.0	30.3
-2	6	5	13.2	14.4
-6	6	5	12.1	-12.6
-7	5	5	8.1	-7.0
-3	5	5	15.0	14.9
1	5	5	6.2	5.5
3	5	5	8.0	-8.4
5	5	5	13.1	-13.4
6	4	5	10.9	10.2
4	4	5	24.1	23.9
2	4	5	6.5	6.7
0	4	5	15.8	16.7
-4	4	5	9.8	-9.3
-6	4	5	9.7	9.4
-5	3	5	21.5	-20.7

Table 8. Observed (FO) and calculated (FC) structure factors for sample 9. Tpq16-4A.

H	K	L	/FO/	/FC/
2	14	-3	7.7	8.1
3	13	-3	14.2	-13.6
1	13	-3	11.4	-10.7
0	12	-3	17.2	-17.4
2	12	-3	25.8	-24.3
4	12	-3	26.6	-27.5
3	11	-3	12.2	-11.9
1	11	-3	19.6	-18.6
-1	11	-3	8.2	-7.5
-3	11	-3	8.4	7.8
-4	10	-3	9.6	-8.9
-2	10	-3	8.8	-8.1
0	10	-3	7.0	7.4
2	10	-3	14.9	15.1
4	10	-3	9.5	9.3
3	9	-3	8.0	-7.5
1	9	-3	20.9	-20.0
-1	9	-3	25.9	-24.8
-3	9	-3	44.4	-42.6
-5	9	-3	37.9	-36.9
-4	8	-3	11.5	-10.7
-2	8	-3	5.3	-5.1
0	8	-3	6.5	6.6
2	8	-3	25.5	25.8
4	8	-3	13.8	13.6
5	7	-3	14.2	-14.3
3	7	-3	24.7	-25.1
1	7	-3	43.0	-43.6
-1	7	-3	22.0	-22.1
-3	7	-3	11.2	11.5
-6	6	-3	14.8	14.6
-4	6	-3	8.1	8.0
-2	6	-3	34.9	-35.0
0	6	-3	31.2	-33.8
2	6	-3	63.8	-66.0
4	6	-3	64.2	-63.6
6	6	-3	16.8	-17.2
5	5	-3	11.2	-11.2
3	5	-3	52.2	-53.6
1	5	-3	43.8	-45.4
-1	5	-3	13.9	-13.8
-5	5	-3	7.2	7.2
-6	4	-3	11.0	-10.3
-4	4	-3	13.1	-13.1
0	4	-3	10.9	-11.6
2	4	-3	47.1	48.9
4	4	-3	23.4	23.6
7	3	-3	31.2	-30.5
5	3	-3	5.6	-5.7
3	3	-3	6.7	-6.3
[illegible]	3	-3	97.3	-98.5
[illegible]	3	-3	80.6	-81.4
[illegible]	3	-3	66.5	-68.3
[illegible]	3	-3	71.2	-71.5
[illegible]	3	-3	27.5	-28.0
[illegible]	2	-3	23.7	-24.1
[illegible]	2	-3	26.7	-27.8
[illegible]	2	-3	62.7	62.3
[illegible]	2	-3	20.1	21.0
4	2	-3	17.3	18.2
6	2	-3	7.1	6.2
[illegible]	1	-3	7.4	-8.3
[illegible]	1	-3	18.5	-18.3
[illegible]	1	-3	64.0	-65.7
[illegible]	1	-3	80.0	-81.4
[illegible]	1	-3	39.3	-39.2
[illegible]	1	-3	6.0	5.9
[illegible]	0	-3	8.6	-8.8
[illegible]	0	-3	9.8	10.3
[illegible]	0	-3	18.6	19.4
[illegible]	0	-3	42.6	-43.8
0	0	-3	112.7	-112.4
2	0	-3	49.1	-48.9
4	0	-3	82.1	-83.3
6	0	-3	34.3	-33.4
-7	3	-2	7.9	-7.4
-5	3	-2	9.1	8.7
-3	3	-2	32.0	33.6
-1	3	-2	48.3	48.8
[illegible]	3	-2	98.1	97.7
[illegible]	3	-2	50.4	51.3
[illegible]	3	-2	29.5	-29.4
[illegible]	2	-2	7.2	-7.3
4	2	-2	22.4	-22.9
[illegible]	2	-2	40.2	42.0
[illegible]	2	-2	84.8	85.2
[illegible]	2	-2	5.2	4.7
[illegible]	2	-2	10.1	9.2
[illegible]	2	-2	7.0	-7.2
[illegible]	1	-2	36.1	-36.6
[illegible]	1	-2	89.5	-89.3
[illegible]	1	-2	66.8	-67.7
[illegible]	1	-2	18.2	-18.6
[illegible]	1	-2	9.2	9.5
[illegible]	1	-2	6.4	7.9
[illegible]	0	-2	70.3	68.9
[illegible]	0	-2	92.7	93.4
[illegible]	0	-2	41.3	-40.6
[illegible]	0	-2	21.7	-19.5
[illegible]	0	-2	97.4	98.4
-4	0	-2	23.4	23.2
-6	0	-2	28.8	28.6
-8	0	-2	29.7	29.9
-8	2	-2	8.2	-7.8
6	4	-2	14.0	-13.6
2	4	-2	12.6	13.8
0	4	-2	31.8	33.9
-2	4	-2	51.6	53.4
-6	4	-2	10.4	-10.1
-3	5	-2	29.4	-30.0
-1	5	-2	62.3	-64.0
1	5	-2	29.7	-31.7
3	5	-2	15.9	-16.0
5	5	-2	6.1	6.3
7	5	-2	8.3	8.4
6	6	-2	54.8	56.6
4	6	-2	46.7	46.5
0	6	-2	6.7	6.1
-2	6	-2	17.7	16.9
-4	6	-2	25.9	25.0
-6	6	-2	23.8	23.4
-3	7	-2	12.8	-13.0
-1	7	-2	33.2	-34.7
1	7	-2	44.5	-46.2
5	7	-2	10.0	10.3
6	8	-2	9.3	-9.5
2	8	-2	10.2	10.4
0	8	-2	24.7	25.1
-2	8	-2	22.3	22.3
-6	8	-2	7.1	-6.6
-3	9	-2	14.8	15.0
-1	9	-2	31.8	32.4
1	9	-2	63.8	63.6
3	9	-2	18.3	18.4
2	10	-2	8.5	8.6
0	10	-2	20.8	20.8
-2	10	-2	13.8	13.9
-3	11	-2	7.1	-6.8
-1	11	-2	18.3	-17.3
1	11	-2	22.4	-21.5
-3	13	-2	6.3	-6.0
-1	13	-2	14.7	-13.7
0	14	-2	7.5	7.6
-2	14	-2	5.9	6.4
-3	13	-1	7.2	-8.2
-4	12	-1	16.4	-15.9
-2	12	-1	29.3	-32.4
3	11	-1	9.2	9.1
-3	11	-1	15.5	-15.1
-5	11	-1	7.7	-7.9
-4	10	-1	15.2	14.8
-2	10	-1	17.1	16.7
2	10	-1	6.9	-7.0
3	9	-1	69.6	-68.4
1	9	-1	45.8	-46.4
-1	9	-1	5.2	-6.0
-3	9	-1	5.6	6.3
-6	8	-1	7.3	7.1
-4	8	-1	18.3	18.3
-2	8	-1	26.9	27.0
0	8	-1	12.0	11.8
2	8	-1	11.1	-11.8
5	7	-1	10.9	10.9
3	7	-1	11.9	12.2
-3	7	-1	31.1	-31.2
-5	7	-1	17.3	-16.8
-6	6	-1	17.6	-17.3
-4	6	-1	31.8	-32.2
-2	6	-1	81.4	-83.0
0	6	-1	49.6	-51.2
2	6	-1	60.4	61.5
4	6	-1	29.5	29.4
6	6	-1	16.6	-16.9
3	5	-1	25.3	27.0
1	5	-1	20.1	20.9
-1	5	-1	37.6	-39.7
-3	5	-1	27.8	-29.2
-5	5	-1	14.5	-14.2
-6	4	-1	12.1	11.7
-4	4	-1	22.5	22.6
-2	4	-1	53.5	55.7
0	4	-1	38.4	40.1
2	4	-1	27.4	-28.8
5	3	-1	47.1	-46.7
3	3	-1	153.3	-153.9
1	3	-1	119.1	-119.2
-1	3	-1	40.8	40.5
-3	3	-1	6.5	-6.0
-5	3	-1	21.0	-20.6
-7	3	-1	10.5	-10.6
-6	2	-1	6.4	6.6
-4	2	-1	51.9	52.3
-2	2	-1	38.7	40.2
0	2	-1	10.4	10.6
2	2	-1	37.3	38.2
4	2	-1	16.1	-17.1
5	1	-1	6.7	7.0
3	1	-1	26.4	27.4
1	1	-1	16.9	16.0
-1	1	-1	40.6	-41.5
[illegible]	[illegible]	-1	42.4	-44.5
[illegible]	[illegible]	-1	21.2	-21.4
[illegible]	[illegible]	-1	16.1	-16.2
[illegible]	[illegible]	-1	63.7	-65.5
[illegible]	[illegible]	-1	98.8	-98.0
[illegible]	[illegible]	-1	51.7	-51.7
2	[illegible]	-1	57.1	55.2
4	[illegible]	-1	62.6	61.9
6	[illegible]	-1	18.4	-18.4
8	[illegible]	-1	27.0	-27.6
7	[illegible]	0	24.5	24.1
[illegible]	[illegible]	0	64.4	63.6
[illegible]	[illegible]	0	50.7	51.1
[illegible]	[illegible]	0	57.4	-55.3
[illegible]	[illegible]	0	10.0	10.1
[illegible]	[illegible]	0	15.9	16.0
[illegible]	[illegible]	0	32.6	33.1
[illegible]	[illegible]	0	38.1	39.3
[illegible]	[illegible]	0	42.4	-41.4
[illegible]	[illegible]	0	12.9	-13.0
[illegible]	[illegible]	0	18.9	-19.2
[illegible]	[illegible]	0	5.8	5.8
[illegible]	[illegible]	0	35.8	35.0
[illegible]	[illegible]	0	6.3	6.9
[illegible]	[illegible]	0	8.0	7.4
[illegible]	[illegible]	0	119.4	119.5
[illegible]	4	0	6.3	6.5
[illegible]	4	0	25.7	24.7
4	4	0	18.8	18.8
[illegible]	4	0	37.4	38.7
7	[illegible]	0	11.8	-11.7
[illegible]	[illegible]	0	17.6	-17.6
[illegible]	[illegible]	0	10.7	10.9
[illegible]	[illegible]	0	16.7	18.0
[illegible]	[illegible]	0	90.9	93.5
[illegible]	[illegible]	0	152.2	153.4
[illegible]	[illegible]	0	6.2	-7.3
[illegible]	[illegible]	0	9.1	-8.9
[illegible]	[illegible]	0	6.6	-6.9
[illegible]	[illegible]	0	27.2	28.9
[illegible]	[illegible]	0	14.1	13.9
[illegible]	[illegible]	0	12.7	12.3
[illegible]	[illegible]	0	4.0	-4.2
[illegible]	[illegible]	0	31.0	32.4
[illegible]	[illegible]	0	34.0	33.0
[illegible]	[illegible]	0	28.9	-29.4
[illegible]	[illegible]	0	10.0	9.8
[illegible]	[illegible]	0	7.4	-7.5
[illegible]	[illegible]	0	14.5	13.8
[illegible]	12	0	55.4	56.0
5	9	1	6.8	-7.5
7	1	2	6.1	5.3
7	7	2	6.2	5.4
5	9	2	11.9	11.7
4	12	2	7.7	7.6
2	12	3	11.6	-11.4
2	4	3	4.0	-4.5
-7	3	4	32.6	32.6
-5	3	4	33.0	32.3
-3	3	4	32.5	34.2
-1	3	4	42.6	43.9
1	3	4	43.6	-43.9
3	3	4	36.7	-37.3
5	3	4	21.5	21.6
7	3	4	31.3	32.2
6	2	4	13.3	13.3
4	2	4	9.6	-9.6
-2	2	4	22.0	-22.9
-4	2	4	34.9	35.2
-6	2	4	20.2	19.4
-7	1	4	13.5	-13.2
-5	1	4	29.8	-29.5
-3	1	4	34.5	-34.7
-1	1	4	16.7	-16.3
1	1	4	11.4	11.2
5	1	4	9.9	-9.5
7	1	4	9.6	-9.9
6	0	4	8.7	-8.1
4	0	4	78.6	77.7
2	0	4	127.0	126.7
0	0	4	64.2	61.1
-2	0	4	82.2	81.5
-4	0	4	18.3	17.1
-6	0	4	6.4	-6.1
6	4	4	7.5	7.5
4	4	4	9.5	9.4
2	4	4	22.1	-21.8
0	4	4	23.7	-24.9
-2	4	4	25.3	25.2
-4	4	4	16.4	16.3
-6	4	4	15.7	15.0
-7	5	4	10.4	-12.0
-5	5	4	19.8	-19.6
-3	5	4	28.0	-27.8
-1	5	4	13.1	-13.0
1	5	4	21.8	22.6
5	5	4	10.2	-9.5
7	5	4	7.6	-7.0
4	6	4	41.0	41.0
2	6	4	95.2	97.2

H	K	L	/FO/	/FC/
0	4	9	25.4	-25.8
4	4	9	9.7	9.6
3	3	9	33.7	-33.0
1	3	9	64.8	-62.7
-1	3	9	71.0	-70.5
-3	3	9	61.8	-60.4
-5	3	9	24.1	-23.0
-7	3	9	9.0	9.5
-6	2	9	16.9	17.3
-2	2	9	26.8	-26.1
6	2	9	9.7	9.7
5	1	9	11.7	-12.4
3	1	9	15.5	-15.2
-1	1	9	7.8	6.5
-5	1	9	15.1	-15.6
-7	1	9	13.0	-13.0
-6	0	9	37.9	-37.6
-2	0	9	17.4	17.8
0	0	9	20.1	-19.2
4	0	9	14.3	-12.8
6	0	9	28.5	-29.7
-5	3	10	11.0	-10.6
1	3	10	14.7	13.6
3	3	10	42.5	42.0
5	3	10	23.4	25.1
4	2	10	8.3	8.3
2	2	10	24.0	24.0
0	2	10	15.9	14.6
-2	2	10	15.3	-15.8
-4	2	10	5.7	-6.1
-5	1	10	7.2	7.2
-3	1	10	7.2	6.9
-1	1	10	9.8	-8.9
1	1	10	19.0	-17.7
3	1	10	18.2	-17.7
5	1	10	8.5	-8.8
4	0	10	8.4	-7.6
0	0	10	43.3	41.9
-2	0	10	64.9	63.7
-4	0	10	35.6	36.4
-6	0	10	29.8	30.5
4	4	10	16.3	16.0
2	4	10	12.8	12.6
0	4	10	8.3	8.1
-4	4	10	15.8	-15.7
-5	5	10	9.3	8.6
-1	5	10	10.2	-10.0
1	5	10	10.7	-9.9
3	5	10	14.8	-14.9
5	5	10	8.7	-8.7

H	K	L	/FO/	/FC/
4	6	10	13.6	-13.3
0	6	10	32.5	33.1
-2	6	10	32.3	32.1
-4	6	10	33.7	34.1
-6	6	10	22.9	23.4
-3	7	10	7.7	7.8
1	7	10	16.2	-16.0
3	7	10	9.9	-10.1
4	8	10	8.6	9.1
2	8	10	8.5	9.1
-4	8	10	10.4	-10.0
1	9	10	14.4	14.8
3	9	10	23.1	24.1
2	10	10	7.6	7.1
-4	10	10	6.8	-6.8
1	11	10	7.9	-8.1
-2	10	11	7.3	7.1
0	10	11	9.9	10.1
1	9	11	12.9	13.1
-3	9	11	14.6	-14.8
-2	8	11	11.0	11.1
0	8	11	14.7	16.0
2	8	11	8.9	9.1
3	7	11	6.4	-6.1
1	7	11	11.2	-12.1
-1	7	11	7.2	-7.1
-3	7	11	8.8	-8.1
-2	6	11	13.3	-13.1
0	6	11	41.0	-42.1
2	6	11	23.5	-24.1
1	5	11	12.5	-13.1
-1	5	11	18.4	-19.1
-2	4	11	18.3	18.1
0	4	11	27.7	28.1
2	4	11	10.5	10.1
3	3	11	24.4	-25.1
1	3	11	11.5	-11.1
-3	3	11	19.8	18.1
-5	3	11	34.3	-33.1
-7	3	11	28.4	-27.1
-6	2	11	15.2	-16.1
-4	2	11	8.4	-8.1
-2	2	11	10.7	11.1
0	2	11	17.6	17.1
2	2	11	21.0	19.1
3	1	11	20.0	20.1
1	1	11	5.3	-4.1
-1	1	11	18.6	-17.1
-2	0	11	21.1	-19.1
			15.1	-13.1

H	K	L	/FO/	/FC/
0	0	11	45.6	-44.3
2	0	11	44.4	-42.8
4	0	11	8.4	8.5
-1	3	11	5.5	4.2
-5	3	12	14.0	14.7
-3	3	12	43.3	43.0
-1	3	12	44.6	43.1
3	3	12	17.3	-18.0
0	2	12	7.1	7.2
-2	2	12	29.3	29.2
-4	2	12	16.3	17.1
-5	1	12	7.4	-7.8
-3	1	12	13.8	-13.6
-1	1	12	14.1	-13.1
3	1	12	10.4	10.8
4	0	12	26.9	28.2
2	0	12	51.1	50.6
0	0	12	32.6	30.9
-2	0	12	19.7	-19.0
-6	0	12	21.8	24.0
0	4	12	18.8	19.3
-2	4	12	14.8	15.8
-4	4	12	13.3	14.3
-6	4	12	8.0	7.9
-5	5	12	7.8	-7.9
-3	5	12	7.7	-8.2
-1	5	12	10.3	-11.4
3	5	12	10.3	11.0
2	6	12	39.2	40.6
0	6	12	11.6	11.9
-2	6	12	7.3	-7.7
-3	7	12	12.5	-12.9
-1	7	12	6.1	-7.1
0	8	12	9.6	9.9
-2	8	12	12.0	11.7
-4	8	12	9.1	9.0
-3	9	12	29.8	30.8
-1	9	12	22.6	25.3
-2	10	12	9.0	9.9
-1	9	13	23.3	-26.0
1	7	13	8.3	9.8
-4	6	13	23.7	-25.7
-2	6	13	7.6	8.6
0	6	13	17.3	18.0
-1	5	13	7.2	7.7
-3	5	13	9.9	-10.0
-4	4	13	13.0	14.0
0	4	13	6.1	-6.2
3	3	13	9.2	-10.6
1	3	13	36.0	-36.5

H	K	L	/FO/	/FC/
-1	3	13	52.0	-51.3
-3	3	13	12.4	-12.3
-5	3	13	13.5	13.8
-6	2	13	8.8	9.2
-4	2	13	7.3	7.7
-2	2	13	9.7	10.3
0	2	13	9.2	-8.9
1	1	13	7.8	7.7
-3	1	13	7.7	-7.5
-5	1	13	10.2	-11.0
-6	0	13	24.0	-25.7
-4	0	13	24.5	-24.6
0	0	13	28.2	27.0
4	0	13	13.9	-15.3
-3	3	14	17.8	-18.4
1	3	14	11.7	11.8

H	K	L	/FO/	/FC/
-2	2	14	9.4	-9.1
-4	2	14	8.8	-8.1
1	1	14	8.8	-8.1
3	1	14	11.3	-11.2
2	0	14	7.6	7.9
0	0	14	7.7	7.6
-2	0	14	35.9	36.9
-4	0	14	40.9	41.6
2	4	14	9.6	10.3
-2	4	14	9.5	-9.8
1	5	14	7.5	-7.6
0	6	14	10.1	10.8
-2	6	14	25.8	28.9
-4	6	14	23.0	28.4
-2	6	15	14.1	-15.5
-1	5	15	10.2	-10.7

H	K	L	/FO/	/FC/
1	3	15	7.6	-8.3
-1	3	15	7.6	-8.0
-3	3	15	9.6	-11.0
-4	2	15	5.9	-6.2
0	2	15	13.6	14.4
1	1	15	12.0	-12.8
-1	1	15	12.8	-13.5
-2	0	15	12.4	-11.9
0	0	15	20.1	-21.9
2	0	15	14.8	-15.8
-1	3	16	14.7	16.3
0	2	16	6.5	6.4
-3	1	16	9.5	-10.6
-1	1	16	8.9	-9.7
-2	0	16	7.4	8.4

Table 8. Observed (FO) and calculated (FC) structure factors for sample 10. Tpt17-1.

H	K	L	/FO/	/FC/
1	3	-5	127.4	-127.5
2	6	4	106.2	104.9
-1	1	-1	40.6	-44.0
1	1	0	31.2	32.2
-1	1	2	67.5	-67.4
-1	1	3	80.8	-77.8
-1	1	4	19.2	-19.9
-1	1	5	10.5	9.3
-1	1	6	9.7	-10.1
-1	1	7	40.1	-40.5
-1	1	8	16.8	-17.4
-1	1	10	11.1	-11.8
-1	1	11	21.0	-21.5
-1	1	12	14.7	-14.2
-1	1	13	6.9	6.9
-1	1	15	17.5	-17.2
-1	1	16	12.7	-12.4
-1	3	-1	38.7	37.0
1	3	0	49.7	-49.4
-1	3	1	117.9	-117.1
-1	3	2	96.1	94.3
-1	3	3	110.2	-109.7
-1	3	4	45.7	47.5
-1	3	6	51.5	53.2
-1	3	7	23.5	23.4
-1	3	8	18.0	-19.4
-1	3	9	72.2	-74.0
-1	3	12	49.5	49.0
-1	3	13	61.3	-61.1
-1	3	15	10.6	-10.2
-1	3	16	20.4	19.6
-1	5	-1	41.9	-40.8
1	5	0	14.8	15.2
-1	5	1	18.1	18.7
-1	5	2	31.8	-30.9
-1	5	3	46.8	-46.6
-1	5	4	16.1	-15.2
-1	5	6	12.3	-12.5
-1	5	7	20.3	-20.6
-1	5	9	6.0	6.1
-1	5	10	13.1	-13.3
-1	5	11	22.2	-22.2
-1	5	12	12.5	-12.8
-1	5	13	10.0	10.0
-1	5	15	14.1	-14.2
1	7	0	28.7	29.6
-1	7	2	49.0	-50.2
-1	7	3	47.7	-48.1
-1	7	5	24.5	24.9
-1	7	7	34.5	-35.0

H	K	L	/FO/	/FC/
-1	7	8	18.7	-20.0
-1	7	12	8.4	-8.1
-1	9	-1	8.1	-8.5
1	9	0	31.4	-31.8
-1	9	1	48.5	-50.4
-1	9	2	70.4	71.1
-1	9	3	25.7	-26.5
-1	9	4	8.4	9.1
-1	9	6	82.5	-83.2
-1	9	7	25.3	25.4
-1	9	8	24.1	25.5
-1	9	9	40.1	-40.4
-1	9	10	6.7	-6.7
-1	9	12	31.2	32.1
-1	9	13	36.4	-34.9
-1	11	0	16.9	17.4
-1	11	1	28.0	-27.9
-1	11	2	24.3	-24.4
-1	11	3	17.3	17.6
-1	11	7	19.5	-20.3
-1	11	8	11.7	-11.5
-1	13	-1	11.1	-11.7
-1	13	0	9.9	9.7
-1	13	1	8.1	8.0
-1	13	2	8.4	-8.5
-1	13	3	14.8	-14.3
-1	13	7	10.0	-10.1
-1	13	-7	11.3	-11.3
-1	13	-6	11.1	-11.2
-1	13	-4	11.9	11.6
-1	13	-2	18.2	-19.0
-1	11	-10	12.4	-13.8
-1	11	-8	10.0	-10.0
-1	11	-3	11.4	-11.3
-1	11	-2	21.8	-20.7
-1	9	0	17.4	17.5
-1	9	-1	19.0	18.4
-1	9	-2	31.4	-32.8
-1	9	-3	13.4	-13.6
-1	9	-4	31.3	-30.0
-1	9	-5	83.6	85.3
-1	9	-6	45.7	-46.6
-1	9	-8	7.9	-7.0
-1	7	-1	29.7	-29.6
-1	7	-10	30.2	31.9
-1	7	-9	13.1	13.3
-1	7	-8	14.0	-14.9
			20.2	-21.1
			7.7	-8.0
			8.2	7.9

H	K	L	/FO/	/FC/
-1	7	-7	8.3	-8.5
-1	7	-6	14.9	-14.5
-1	7	-3	26.1	-26.1
-1	7	-2	36.2	-36.4
-1	5	-14	11.4	-11.5
-1	5	-11	13.5	-14.2
-1	5	-10	12.0	-12.5
-1	5	-7	29.4	-30.1
-1	5	-6	32.9	-33.8
-1	5	-4	20.3	20.5
-1	5	-3	16.2	-15.8
-1	5	-2	64.8	-65.2
-1	3	-15	12.6	-12.0
-1	3	-14	17.3	16.1
-1	3	-13	41.5	-43.1
-1	3	-11	19.7	20.1
-1	3	-10	13.7	13.9
-1	3	-9	67.0	-67.4
-1	3	-8	16.4	-17.0
-1	3	-7	37.2	-38.4
-1	3	-6	125.9	129.5
-1	3	-4	39.6	-38.8
-1	3	-3	85.3	-84.4
-1	3	-2	40.5	39.2
-1	1	-15	16.8	-16.2
-1	1	-14	13.7	-12.6
-1	1	-13	9.2	9.3
-1	1	-11	18.2	-18.6
-1	1	-10	20.0	-20.8
-1	1	-7	30.0	-30.3
-1	1	-6	34.3	-33.9
-1	1	-3	40.2	-41.4
-1	1	-2	86.9	-84.4
0	14	4	7.4	-7.7
0	14	2	9.0	10.0
0	12	8	31.9	31.5
0	12	7	28.2	-27.9
0	12	5	19.0	19.1
0	12	4	28.3	29.3
0	12	3	21.1	-21.8
0	12	1	19.7	-20.3
0	12	0	69.7	70.9
0	10	12	8.5	8.0
0	10	11	13.3	14.2
0	10	10	6.2	6.4
0	10	9	10.7	-10.0
0	10	7	18.1	18.9
0	10	6	19.2	19.1
0	10	4	8.1	-8.5
0	10	3	8.1	8.5

H	K	L	/FO/	/FC/
0	10	2	23.6	23.8
0	10	0	6.4	-6.8
0	8	12	12.2	13.2
0	8	11	20.0	20.6
0	8	9	14.7	-15.6
0	8	8	8.9	-8.8
0	8	7	29.0	29.3
0	8	6	31.3	31.1
0	8	4	15.2	-15.4
0	8	2	26.0	25.9
0	8	1	14.5	14.8
0	6	14	12.5	12.5
0	6	13	23.0	22.8
0	6	12	16.8	15.8
0	6	11	50.0	-49.4
0	6	10	37.3	38.9
0	6	8	66.6	68.0
0	6	7	56.9	-56.6
0	6	6	6.5	-7.6
0	6	5	38.1	38.0
0	6	4	71.3	69.8
0	6	3	30.6	-31.3
0	6	2	11.6	13.7
0	6	1	53.1	-55.2
0	6	0	155.1	157.9
0	4	13	6.1	-6.0
0	4	12	24.2	23.4
0	4	11	31.9	32.0
0	4	10	8.8	8.5
0	4	9	26.0	-27.9
0	4	8	14.5	-14.4
0	4	7	44.6	46.7
0	4	6	59.1	61.4
0	4	5	18.0	18.7
0	4	4	23.1	-23.4
0	4	3	14.1	-14.5
0	4	2	30.0	31.3
0	4	1	41.7	43.7
0	4	0	44.9	45.1
0	2	15	18.2	18.5
0	2	13	9.8	-10.1
0	2	12	7.9	7.4
0	2	11	21.8	21.4
0	2	10	16.5	17.3
0	2	7	38.7	38.7
0	2	6	22.9	23.4
0	2	5	8.3	-7.5
0	2	3	62.3	59.8
0	2	2	82.1	81.5

H	K	L	/FO/	/FC/
0	2	0	34.1	-36.6
0	0	15	28.2	-27.7
0	0	13	33.3	32.7
0	0	12	40.1	38.2
0	0	11	47.7	-48.4
0	0	10	44.6	45.1
0	0	9	23.7	-26.2
0	0	8	74.0	74.4
0	0	7	57.5	-57.6
0	0	6	39.6	39.9
0	0	5	102.4	102.2
0	0	4	53.6	54.2
0	0	3	107.9	-106.2
0	0	1	58.1	-53.8
1	3	5	102.4	-104.2
2	14	2	8.1	8.6
2	12	1	13.1	13.0
2	12	8	21.5	21.7
2	12	5	11.0	-11.4
2	12	4	14.0	-12.9
2	12	3	49.3	48.3
2	12	2	16.3	-15.1
2	12	1	10.7	10.4
2	12	0	41.0	-40.5
2	12	-1	39.3	39.2
2	10	10	23.6	23.5
2	10	8	10.7	10.1
2	10	6	11.1	-12.1
2	10	5	26.8	26.0
2	10	4	12.7	11.6
2	10	3	9.7	-9.4
2	10	2	9.6	-10.2
2	10	1	14.6	15.2
2	8	11	21.0	20.3
2	8	10	10.9	11.8
2	8	8	11.0	11.7
2	8	7	11.5	-10.3
2	8	6	7.5	8.7
2	8	5	27.3	27.5
2	8	4	11.5	11.0
2	8	3	14.4	-12.7
2	8	2	26.2	25.7
2	8	1	29.2	30.4
2	8	-1	11.4	-11.6
2	6	12	55.0	54.0
2	6	11	26.8	-27.7
2	6	9	7.4	-6.8
2	6	8	38.5	38.7
2	6	6	9.5	-9.1
2	6	5	14.7	-14.8

H	K	L	/FO/	/FC/
2	6	3	40.5	-41.9
2	6	2	21.5	22.0
2	6	1	86.2	-86.0
2	6	0	99.9	100.6
2	6	-1	64.2	65.1
2	4	14	15.3	13.8
2	4	11	12.9	12.6
2	4	10	15.4	14.2
2	4	7	19.1	19.0
2	4	6	40.4	39.7
2	4	5	8.1	8.1
2	4	4	21.8	-20.3
2	4	2	54.8	55.5
2	4	1	56.1	56.6
2	4	-1	27.5	-26.9
2	2	13	9.7	-8.9
2	2	11	32.0	30.7
2	2	10	26.2	26.8
2	2	8	32.5	-32.2
2	2	6	61.5	60.2
2	2	5	49.1	51.1
2	2	3	28.2	-28.4
2	2	1	40.5	39.7
2	2	0	46.8	45.0
2	2	-1	45.0	43.7
2	0	15	20.9	-19.8
2	0	12	61.7	61.9
2	0	11	48.6	-48.9
2	0	8	74.0	74.2
2	0	7	18.0	19.4
2	0	6	22.2	-22.9
2	0	5	52.3	-53.1
2	0	4	128.4	128.2
2	0	3	45.7	-48.1
2	0	2	112.1	109.9
2	0	1	97.1	-94.7
2	0	0	118.2	118.5
2	0	-1	51.0	50.0
2	0	-2	39.7	-37.1
2	0	-3	41.6	-40.0
2	0	-4	86.2	84.2
2	0	-5	40.5	39.3
2	0	-6	103.2	104.3
2	0	-7	127.2	-129.8
2	0	-8	36.6	38.0
2	0	-9	15.7	17.0
2	0	-10	66.3	67.6
2	0	-11	13.3	-13.9
2	0	-12	21.0	-20.3
2	0	-14	43.5	42.9

Sample 10. Tpt17-1 (continued)

H	K	L	/FO/	/FC/
4	10	-8	13.7	14.6
4	10	-10	7.4	-7.5
4	12	-2	26.9	27.5
4	12	-3	40.2	-38.3
4	12	-4	9.9	8.6
4	12	-5	10.4	-9.3
4	12	-6	42.8	43.3
4	12	-7	11.9	-11.8
5	1	-1	6.8	6.3
5	1	0	22.1	-21.0
5	1	1	23.7	-24.4
5	1	4	12.3	-12.7
5	1	5	24.6	-23.2
5	1	7	11.4	11.2
5	1	9	15.7	-16.8
5	1	10	11.3	-12.4
5	3	-1	53.7	-52.2
5	3	0	74.7	72.7
5	3	1	29.3	-28.0
5	3	2	10.0	9.8
5	3	3	85.7	-85.2
5	3	4	28.0	26.5
5	3	5	24.0	25.2
5	3	7	41.1	-41.9
5	3	8	6.7	-6.3
5	3	10	33.7	33.1
5	3	11	36.6	-36.3
5	5	0	20.4	-20.6
5	5	1	17.3	-16.4
5	5	3	7.5	7.0
5	5	4	13.6	-13.4
5	5	5	23.1	-23.4
5	5	7	12.3	12.9
5	5	9	13.3	-13.3
5	5	10	12.4	-12.7
5	7	-1	13.4	13.9
5	7	0	9.5	-9.8
5	7	1	22.0	-21.5
5	7	2	6.7	-6.4
5	7	5	9.6	-10.3
5	7	8	7.9	-8.3
5	7	9	13.3	-13.7
5	9	-1	40.9	-40.7
5	9	0	42.1	41.4
5	9	1	11.1	-10.5
5	9	2	16.5	15.9
5	9	3	48.0	-49.4
5	9	4	13.0	13.1
5	9	5	11.0	11.1
5	9	7	22.0	-22.2
5	11	-1	9.3	11.1
5	11	1	10.9	-11.6
5	11	-7	7.5	6.7
5	11	-6	10.3	12.4
5	11	-4	19.4	-20.0
5	11	-3	11.6	-11.9
5	9	-9	13.1	-13.5
5	9	-8	41.1	42.6
5	9	-7	37.6	-38.3
5	9	-6	9.5	-10.3
5	9	-5	14.4	-13.8
5	9	-4	30.5	31.5
5	9	-2	24.2	-24.1
5	7	-9	18.4	-18.2
5	7	-8	15.1	-15.8
5	7	-7	8.0	7.3
5	7	-6	17.8	17.2
5	7	-4	32.4	-31.1
5	7	-3	18.5	-19.5
5	7	-2	12.2	12.5
5	5	-13	14.0	-14.7
5	5	-12	10.2	-10.5
5	5	-10	11.7	11.1
5	5	-9	12.1	-12.3
5	5	-8	22.5	-23.8
5	5	-6	9.7	10.1
5	5	-4	22.2	-22.3
5	5	-3	13.0	-13.9
5	3	-13	16.9	17.9
5	3	-12	18.7	19.0
5	3	-11	34.5	-33.8
5	3	-10	12.1	-13.7
5	3	-9	30.3	-30.2
5	3	-8	69.0	66.9
5	3	-7	49.5	-47.7
5	3	-6	8.0	-7.4
5	3	-5	33.1	-30.7
5	3	-4	34.3	33.1
5	3	-3	8.0	-8.9
5	3	-2	33.5	-31.5
5	1	-13	13.1	-13.9
5	1	-12	9.0	-9.6
5	1	-10	8.5	8.1
5	1	-9	18.2	-18.8
5	1	-8	26.5	-26.0
5	1	-6	14.5	15.1
5	1	-4	32.7	-33.4
5	1	-3	21.0	-21.5
5	1	-2	8.6	8.7
6	10	2	8.7	-8.5
6	10	0	13.6	14.3
6	8	5	14.2	14.5
6	8	2	9.8	-8.7
6	8	1	10.4	10.8
6	8	0	21.7	20.5
6	6	6	34.1	33.3
6	6	5	28.7	-29.0
6	6	3	21.0	19.2
6	6	2	30.9	30.8
6	6	1	24.2	-23.0
6	6	-1	21.2	-21.2
6	4	5	21.1	21.4
6	4	4	9.4	9.3
6	4	3	13.6	-13.9
6	4	2	13.7	-12.7
6	4	1	17.7	16.6
6	4	0	31.9	32.7
6	4	-1	8.1	7.7
6	2	9	13.7	15.0
6	2	7	9.8	-9.7
6	2	5	17.4	18.3
6	2	4	18.0	18.5
6	2	2	9.0	-8.3
6	2	1	7.6	7.3
6	2	0	18.7	18.4
6	0	9	42.5	-42.9
6	0	8	19.9	19.5
6	0	6	52.3	52.4
6	0	5	30.8	-30.7
6	0	4	10.8	-10.3
6	0	3	9.7	9.8
6	0	2	33.3	35.2
6	0	1	18.1	-17.6
6	0	0	12.6	14.1
6	0	-1	21.3	-21.9
6	0	-2	80.4	81.4
6	0	-3	43.0	-42.7
6	0	-5	14.8	-16.0
6	0	-6	54.7	54.9
6	0	-7	27.5	26.4
6	0	-8	14.1	-13.8
6	0	-9	47.6	-47.8
6	0	-10	38.1	38.8
6	0	-12	33.8	33.0
6	0	-13	33.2	-33.4
6	2	-3	8.8	9.4
6	2	-4	22.0	23.6
6	2	-6	13.4	-13.6
6	2	-8	20.9	20.0
6	2	-9	20.5	22.6
6	2	-11	12.3	-11.8
6	2	-13	10.9	12.5
6	4	-2	16.7	-17.0
6	4	-3	7.5	-8.2
6	4	-4	18.7	18.3
6	4	-5	17.5	17.2
6	4	-8	7.6	7.2
6	4	-9	8.6	7.8
6	4	-12	11.2	12.4
6	6	-2	72.5	73.8
6	6	-3	20.6	-21.2
6	6	-5	23.6	-23.3
6	6	-6	31.9	30.7
6	6	-7	19.7	19.4
6	6	-9	28.3	-28.9
6	6	-10	32.7	32.4
6	8	-2	13.5	-13.1
6	8	-4	13.9	14.0
6	8	-5	10.2	11.4
6	8	-9	8.2	8.4
6	10	-4	9.1	10.5
7	1	-1	5.7	-6.5
7	1	0	15.9	-17.0
7	1	4	14.4	-14.3
7	1	6	8.0	8.0
7	3	0	30.9	32.4
7	3	1	14.5	-15.1
7	3	2	9.3	-10.1
7	3	3	40.6	-39.5
7	3	4	44.6	44.2
7	3	5	14.5	-14.5
7	5	0	15.2	-16.4
7	5	4	9.7	-10.0
7	7	-1	7.0	-7.3
7	7	0	9.6	-9.2
7	7	-4	8.5	-9.0
7	5	-9	13.3	-14.4
7	5	-7	11.2	11.3
7	5	-5	18.0	-16.7
7	5	-4	15.6	-17.4
7	5	-2	12.0	11.9
7	3	-11	22.0	-22.6
7	3	-9	11.6	11.2
7	3	-8	13.1	13.5
7	3	-7	50.7	-50.5
7	3	-6	15.4	16.4
7	3	-5	10.9	-10.7
7	3	-4	40.7	42.2
7	3	-3	43.4	-41.7
7	3	-2	23.2	-24.2
7	1	-11	6.6	7.4
7	1	-9	18.2	-18.1
7	1	-7	10.5	9.8
7	1	-5	15.8	-16.1
7	1	-4	17.5	-18.0
7	1	-2	9.6	9.6
8	4	0	9.3	8.8
8	4	-1	7.1	7.7
8	2	2	14.2	-13.0
8	2	0	15.8	16.2
8	2	-1	17.1	18.4
8	0	3	12.1	-13.2
8	0	2	45.4	45.4
8	0	1	10.4	-10.0
8	0	0	9.3	10.0
8	0	-1	39.4	-40.2
8	0	-2	29.0	29.3
8	0	-3	19.5	19.7
8	0	-5	22.5	-22.3
8	0	-6	9.5	10.9
8	0	-8	27.7	28.4
8	2	-3	12.5	-13.1
8	2	-5	12.0	13.0
8	2	-6	7.3	7.3
8	4	-4	9.0	9.2
8	4	-5	12.3	13.3

Table 8. Observed (FO) and calculated (FC) structure factors for sample 11. Tas22-1a.

H	K	L	/FO/	/FC/
2	12	-1	19.1	16.4
0	12	-1	13.6	-13.4
-2	12	-1	28.0	-26.4
-3	11	-1	13.8	-12.7
-2	10	-1	14.9	14.4
-4	10	-1	12.6	12.1
1	9	-1	40.3	-40.6
0	8	-1	9.6	8.1
-2	8	-1	25.0	24.3
-4	8	-1	18.4	17.9
-5	7	-1	15.3	-14.9
-3	7	-1	29.6	-29.0
2	6	-1	59.2	58.1
0	6	-1	44.2	-44.8
-2	6	-1	78.2	-79.2
-4	6	-1	34.8	-33.7
-6	6	-1	16.6	-15.1
-5	5	-1	13.3	-13.4
-3	5	-1	28.3	-28.9
-1	5	-1	40.6	-40.2
1	5	-1	21.3	21.3
2	4	-1	28.7	-29.7
0	4	-1	34.2	34.3
-2	4	-1	54.9	54.7
-4	4	-1	25.7	26.1
-6	4	-1	11.8	9.6
-5	3	-1	16.3	-17.4
-1	3	-1	49.7	46.8
1	3	-1	125.6	-123.9
2	2	-1	27.5	28.9
-2	2	-1	40.9	43.0
-4	2	-1	50.7	50.7
-5	1	-1	20.3	-20.7
-3	1	-1	42.2	-44.8
-1	1	-1	41.3	-41.6
1	1	-1	16.8	16.6
2	0	-1	56.2	57.2
0	0	-1	43.1	-40.6
-2	0	-1	102.8	-100.6
-4	0	-1	65.6	-64.8
-6	0	-1	17.5	-18.0
2	8	-1	11.6	-11.8
2	10	-1	9.8	-9.0
2	12	0	25.3	23.2
0	12	0	45.3	43.1
1	11	0	10.8	11.8
1	9	0	29.6	-29.6
3	9	0	27.5	26.6
5	9	0	30.0	30.4
6	8	0	12.2	12.6

H	K	L	/FO/	/FC/
4	8	0	13.2	12.1
1	7	0	26.9	27.6
2	6	0	84.4	85.0
0	6	0	150.2	151.8
1	5	0	19.6	19.1
3	5	0	11.5	10.0
5	5	0	19.9	-19.0
6	4	0	24.3	22.9
4	4	0	18.8	18.2
0	4	0	31.3	30.1
1	3	0	60.0	-60.4
3	3	0	48.2	47.6
5	3	0	66.9	65.9
7	3	0	24.9	24.9
6	2	0	19.3	19.0
4	2	0	34.0	32.4
2	2	0	30.7	32.0
0	2	0	52.6	-49.6
1	1	0	35.1	36.0
5	1	0	20.2	-21.6
7	1	0	13.9	-13.7
2	0	0	119.5	122.4
-5	9	1	28.3	-26.7
-3	9	1	62.1	-62.2
-4	8	1	8.9	-8.8
-5	7	1	10.9	9.2
-3	7	1	12.0	11.9
-4	6	1	33.8	31.8
-6	6	1	18.5	-17.2
-3	5	1	26.5	27.0
-5	3	1	50.5	-49.0
-3	3	1	158.9	-160.8
-4	2	1	20.5	-21.3
-3	1	1	27.1	28.2
-4	0	1	63.4	63.2
-6	0	1	20.4	-21.3
-0	0	1	30.0	-30.8
-4	12	2	16.4	16.2
1	11	2	13.6	-13.7
-1	11	2	15.3	-16.2
0	10	2	17.4	17.6
2	10	2	15.2	14.1
1	9	2	30.6	29.6
-1	9	2	55.5	55.1
-3	9	2	16.7	15.8
-5	9	2	19.3	-17.9
-2	8	2	11.3	10.6
0	8	2	25.2	25.0
2	8	2	18.5	18.7
1	7	2	31.2	-31.7

H	K	L	/FO/	/FC/
-1	7	2	41.5	-42.2
-5	7	2	11.0	10.2
-6	6	2	55.3	54.2
-4	6	2	45.1	44.8
2	6	2	15.5	16.1
1	5	2	59.9	-61.3
-1	5	2	28.5	-28.8
-3	5	2	16.7	-15.3
-6	4	2	13.7	-14.3
-2	4	2	13.6	13.4
0	4	2	36.3	36.2
2	4	2	48.7	51.2
1	3	2	57.0	56.5
-1	3	2	95.8	93.6
-3	3	2	48.4	48.0
-5	3	2	34.5	-33.2
-7	3	2	20.8	-21.2
-6	2	2	11.1	-12.0
-4	2	2	20.4	-21.9
-2	2	2	38.7	40.0
0	2	2	91.8	88.9
2	2	2	10.6	10.0
1	1	2	93.3	-91.4
-1	1	2	64.1	-66.0
-3	1	2	16.2	-19.2
-8	0	2	24.0	22.0
-6	0	2	73.9	73.2
-4	0	2	86.6	89.5
-2	0	2	43.6	-43.8
0	0	2	39.3	-33.0
2	0	2	92.9	90.7
-2	12	3	18.1	-18.5
-4	12	3	21.9	-21.0
-1	11	3	14.9	-14.1
-2	10	3	13.9	14.4
-1	9	3	14.7	-13.7
1	9	3	19.1	-18.9
0	8	3	9.2	8.8
-2	8	3	21.8	22.1
-4	8	3	12.5	12.7
-5	7	3	12.3	-12.3
-3	7	3	23.0	-22.6
-1	7	3	37.8	-39.1
1	7	3	18.6	-18.5
2	6	3	27.7	-30.1
0	6	3	35.7	-34.3
-2	6	3	59.5	-59.2
-4	6	3	58.1	-58.0
-6	6	3	18.0	-16.5
-5	5	3	12.2	-10.4

H	K	L	/FO/	/FC/
-3	5	3	49.4	-49.5
-1	5	3	40.7	-42.1
1	5	3	11.0	-11.3
-2	4	3	47.9	47.6
-4	4	3	25.1	23.9
-7	3	3	29.7	-28.9
-1	3	3	84.7	-85.6
1	3	3	77.6	-76.4
2	2	3	25.8	-27.6
0	2	3	63.1	62.5
-2	2	3	24.3	24.7
-4	2	3	18.5	20.2
-5	1	3	17.5	-17.4
-3	1	3	61.3	-63.6
-1	1	3	79.4	-80.2
1	1	3	35.3	-35.2
2	0	3	41.5	-43.1
0	0	3	126.3	-117.9
-2	0	3	51.4	-52.1
-4	0	3	80.9	-82.2
-6	0	3	30.2	-29.7
-8	0	3	16.3	15.5
0	12	4	16.0	18.2
2	12	4	30.3	29.8
-3	9	4	16.0	15.7
-5	9	4	19.3	20.9
-4	8	4	13.2	12.8
0	8	4	11.5	-11.6
-3	7	4	11.5	-11.1
-5	7	4	18.3	-19.2
-4	6	4	15.1	15.2
-2	6	4	22.3	21.9
0	6	4	64.3	61.8
2	6	4	89.8	91.5
1	5	4	22.7	24.5
-1	5	4	10.5	-11.0
-3	5	4	25.4	-24.8
-5	5	4	17.4	-17.1
-6	4	4	15.2	16.0
-4	4	4	20.6	19.4
-2	4	4	22.9	23.0
0	4	4	23.2	-24.3
2	4	4	21.8	-23.1
1	3	4	49.5	-49.0
-1	3	4	41.1	41.8
-3	3	4	38.8	38.8
-5	3	4	33.1	34.4
-7	3	4	30.7	33.2
-6	2	4	20.3	19.9
-4	2	4	33.4	35.1

H	K	L	/FO/	/FC/
-2	2	4	18.2	-16.4
1	1	4	13.2	15.2
-1	1	4	13.3	-12.2
-3	1	4	30.1	-31.0
-5	1	4	25.7	-26.7
-7	1	4	12.4	-12.2
-4	0	4	14.9	15.0
-2	0	4	77.5	77.8
0	0	4	64.6	65.2
2	0	4	131.5	130.2
-1	11	5	9.5	10.0
-3	9	5	26.1	-24.7
-1	9	5	59.7	-61.3
1	9	5	34.2	-36.4
-1	7	5	21.7	22.1
2	6	5	16.1	-17.0
0	6	5	40.0	39.1
-2	6	5	22.3	22.0
-6	6	5	16.7	-15.7
-3	5	5	18.0	18.0
0	4	5	8.7	9.0
-6	4	5	11.3	10.0
-5	3	5	22.2	-20.0
-3	3	5	65.7	-65.0
-1	3	5	124.3	-124.9
1	3	5	98.7	-99.2
2	2	5	38.0	38.2
0	2	5	13.0	-14.1
-2	2	5	16.2	-17.2
-4	2	5	10.8	10.0
-3	1	5	16.5	18.1
-1	1	5	16.7	16.0
2	0	5	48.7	-47.0
0	0	5	107.3	107.0
-2	0	5	48.9	49.1
-4	0	5	27.7	-30.2
-6	0	5	17.0	-17.0
-8	0	5	15.5	-16.0
-4	12	6	22.0	22.0
-2	12	6	19.3	20.2
0	10	6	12.2	12.0
1	9	6	48.9	49.0
-1	9	6	16.4	16.0
-3	9	6	11.0	-12.7
0	8	6	18.9	19.0
2	8	6	21.2	22.4
1	7	6	13.6	-13.0
-6	6	6	20.5	21.0
-4	6	6	64.4	64.7
-2	6	6	68.5	67.7

H	K	L	/FO/	/FC/
2	6	6	16.6	-18.3
1	5	6	29.3	-31.7
-3	5	6	18.6	18.9
-5	5	6	9.5	9.1
-4	4	6	10.1	-10.1
0	4	6	49.1	50.0
2	4	6	36.7	38.7
1	3	6	125.8	126.4
-1	3	6	44.4	46.2
-3	3	6	38.7	-41.4
-2	2	6	23.5	24.6
0	2	6	23.1	24.4
2	2	6	52.1	54.7
1	1	6	33.0	-34.4
-1	1	6	8.9	-9.7
-3	1	6	16.7	16.9
-5	1	6	12.2	13.8
-6	0	6	39.9	38.4
-4	0	6	93.4	95.0
-2	0	6	95.7	96.2
0	0	6	27.6	26.6
2	0	6	29.7	-31.1
-2	12	7	23.4	-24.7
-5	9	7	25.0	-22.9
-1	9	7	18.7	20.2
1	9	7	16.7	-15.9
0	8	7	19.3	20.8
-2	8	7	16.8	18.5
-3	7	7	15.7	-15.3
-1	7	7	27.3	-28.8
0	6	7	49.0	-51.5
-2	6	7	64.0	-64.8
-4	6	7	17.6	-18.5
-3	5	7	13.8	-15.7
-1	5	7	25.1	-26.1
1	5	7	24.5	-25.7
2	4	7	13.1	13.8
0	4	7	38.7	39.5
-2	4	7	22.6	23.8
-4	4	7	14.5	13.6
-7	3	7	36.2	-37.0
-5	3	7	41.3	-40.2
-1	3	7	27.8	28.4
1	3	7	25.4	-25.8
0	2	7	38.3	38.9
-2	2	7	52.2	55.0
-3	1	7	22.9	-23.5
-1	1	7	40.2	-41.5
1	1	7	27.3	-29.3
2	0	7	11.9	12.1

Table 8. Observed (FO) and calculated (FC) structure factors for sample 12. Tas22-1b.

H	K	L	/FO/	/FC/
7	1	0	13.2	-13.8
5	1	0	19.9	-20.2
3	1	0	7.4	6.7
1	1	0	38.1	42.6
8	2	0	9.2	9.2
6	2	0	18.2	17.9
4	2	0	32.8	33.5
2	2	0	33.4	32.5
0	2	0	45.1	-47.5
7	3	0	24.0	24.6
5	3	0	64.3	62.2
3	3	0	47.5	48.9
1	3	0	60.3	-61.6
8	4	0	7.4	7.0
6	4	0	24.6	23.5
4	4	0	18.7	18.9
0	4	0	30.6	28.6
7	5	0	12.6	-12.2
5	5	0	17.9	-17.9
3	5	0	11.0	11.9
1	5	0	20.5	18.6
2	6	0	92.9	90.3
0	6	0	161.9	161.1
5	7	0	11.6	-11.1
3	7	0	8.1	-7.8
1	7	0	30.0	29.1
7	7	0	7.5	-7.9
6	8	0	12.6	13.2
4	8	0	12.8	12.9
0	8	0	9.0	-8.0
5	9	0	32.4	31.8
3	9	0	31.9	30.5
1	9	0	33.7	-31.8
6	10	0	9.5	9.8
4	10	0	9.3	8.7
0	10	0	7.4	-7.4
1	11	0	13.5	13.6
2	12	0	30.0	29.2
0	12	0	55.5	54.0
1	13	0	7.8	7.6
2	14	1	8.7	8.8
3	13	1	8.6	-8.1
1	13	1	7.3	-7.1
-4	12	1	15.2	14.2
-2	12	1	20.6	20.1
0	12	1	17.3	-16.7
2	12	1	31.4	-31.5
4	12	1	13.6	-14.3
3	11	1	13.9	-14.4
-3	11	1	9.3	9.6

H	K	L	/FO/	/FC/
-2	10	1	9.5	-9.7
2	10	1	17.8	18.1
4	10	1	14.5	13.9
-1	9	1	46.8	-46.4
-3	9	1	71.3	-69.7
-5	9	1	30.5	-30.1
-2	8	1	11.9	-11.2
0	8	1	10.8	9.6
2	8	1	26.1	25.7
4	8	1	21.2	19.8
5	7	1	15.2	-15.8
3	7	1	29.8	-29.8
-3	7	1	12.4	11.9
-5	7	1	9.7	9.3
-7	7	1	6.2	-5.7
-6	6	1	16.5	-16.3
-4	6	1	31.8	32.2
-2	6	1	62.4	60.2
0	6	1	49.6	-49.4
2	6	1	81.2	-80.7
4	6	1	33.3	-32.9
6	6	1	15.8	-15.8
5	5	1	14.7	-14.0
3	5	1	29.5	-28.8
1	5	1	40.6	-40.6
-1	5	1	20.8	20.3
-3	5	1	26.0	26.8
-2	4	1	30.1	-29.4
0	4	1	35.4	35.1
2	4	1	55.5	55.1
4	4	1	26.3	25.6
6	4	1	10.5	11.5
7	3	1	9.0	-9.4
5	3	1	16.2	-16.7
1	3	1	47.7	44.0
-1	3	1	127.7	-127.9
-3	3	1	163.7	-163.0
-5	3	1	49.6	-48.4
-8	2	1	10.9	10.9
-4	2	1	17.4	-18.0
-2	2	1	27.4	27.2
2	2	1	39.8	41.1
4	2	1	50.6	51.5
6	2	1	9.3	9.3
5	1	1	19.4	-20.9
3	1	1	43.8	-43.3
1	1	1	40.5	-44.2
-1	1	1	18.1	18.7
-3	1	1	26.4	26.6
-5	1	1	6.2	5.7

H	K	L	/FO/	/FC/
-7	1	1	7.4	-7.0
-8	0	1	26.7	-26.9
-6	0	1	18.3	-17.8
-4	0	1	60.7	60.5
-2	0	1	60.5	62.7
0	0	1	52.2	-48.6
2	0	1	99.2	-100.4
4	0	1	64.8	-62.5
6	0	1	17.1	-17.4
0	14	2	7.3	7.5
1	13	2	9.0	-8.5
1	13	2	11.2	-12.5
-4	12	2	18.4	19.3
1	11	2	19.6	-20.3
1	11	2	16.6	-16.5
2	10	2	14.8	15.2
0	10	2	19.5	19.5
2	10	2	7.8	8.2
-5	9	2	21.2	-20.7
3	9	2	19.3	18.0
1	9	2	64.2	62.5
1	9	2	33.2	31.7
3	9	2	13.9	15.5
5	9	2	10.2	9.9
2	8	2	21.2	21.1
0	8	2	28.0	27.2
-2	8	2	11.9	12.0
6	8	2	10.1	-10.1
5	7	2	10.8	10.9
1	7	2	46.5	-46.2
1	7	2	34.0	-33.4
3	7	2	12.1	-12.0
6	6	2	23.2	23.9
4	6	2	21.5	22.4
2	6	2	16.7	18.4
4	6	2	49.5	48.4
6	6	2	58.2	56.7
7	5	2	8.3	8.8
5	5	2	16.6	-16.1
1	5	2	28.9	-28.0
1	5	2	62.4	-62.1
3	5	2	28.2	-28.7
1	4	2	7.3	-8.9
4	4	2	51.7	52.3
4	4	2	37.8	38.3
2	4	2	13.5	12.8
6	4	2	14.5	-14.2
7	3	2	20.8	-20.9
5	3	2	35.7	-33.2
3	3	2	47.9	49.5

H	K	L	/FO/	/FC/
-1	3	2	100.1	101.3
1	3	2	57.2	57.0
3	3	2	36.3	36.8
5	3	2	8.0	8.3
8	2	2	6.3	-7.2
4	2	2	9.0	9.9
2	2	2	10.8	12.2
0	2	2	88.8	89.5
-2	2	2	42.0	42.1
-4	2	2	22.1	-22.6
-6	2	2	10.0	-10.8
-7	1	2	8.7	8.3
-3	1	2	18.3	-18.5
-1	1	2	66.1	-69.7
1	1	2	88.4	-90.1
3	1	2	33.5	-34.4
8	0	2	28.9	29.1
6	0	2	29.5	30.2
4	0	2	24.9	23.8
2	0	2	88.4	89.7
0	0	2	31.1	-36.1
-2	0	2	46.9	-43.9
-4	0	2	93.9	92.9
-6	0	2	73.2	72.5
-8	0	2	20.8	20.9
-5	1	2	9.6	9.7
-1	13	3	8.8	-9.6
-3	13	3	10.6	-12.0
-4	12	3	25.6	-26.9
-2	12	3	22.7	-23.1
0	12	3	13.8	-14.9
-1	11	3	16.4	-17.3
-3	11	3	11.9	-12.7
-4	10	3	10.9	10.9
-2	10	3	17.3	16.9
0	10	3	6.9	6.6
5	9	3	36.1	-35.8
3	9	3	39.9	-39.2
1	9	3	22.7	-21.9
-1	9	3	16.6	-18.0
-4	8	3	14.8	14.7
-2	8	3	25.0	24.1
0	8	3	9.9	9.4
4	8	3	9.9	-10.9
3	7	3	11.1	11.7
1	7	3	19.9	-21.2
-1	7	3	42.4	-43.2
-3	7	3	25.6	-25.0
-5	7	3	13.3	-13.7
-6	6	3	17.8	-16.8

H	K	L	/FO/	/FC/
-4	6	3	64.9	-64.0
-2	6	3	66.7	-62.7
0	6	3	37.1	-36.4
2	6	3	30.0	-32.5
4	6	3	11.5	11.5
6	6	3	15.4	15.0
5	5	3	7.3	8.0
1	5	3	12.9	-12.9
-1	5	3	43.2	-44.5
-3	5	3	53.7	-54.6
-5	5	3	12.5	-12.7
-4	4	3	25.3	25.2
-2	4	3	46.2	47.3
0	4	3	6.5	-6.4
2	4	3	5.9	-6.2
4	4	3	12.2	-13.6
7	3	3	26.0	-25.7
5	3	3	69.2	-69.3
3	3	3	67.9	-65.1
1	3	3	79.1	-76.7
-1	3	3	92.5	-91.6
-7	3	3	32.8	-32.0
-8	2	3	9.1	-8.1
-4	2	3	18.6	18.2
-2	2	3	24.8	26.2
0	2	3	60.2	59.5
2	2	3	26.5	-26.1
4	2	3	22.5	-24.1
1	1	3	37.4	-36.6
-1	1	3	84.1	-83.0
-3	1	3	67.3	-67.0
-5	1	3	19.5	-18.9
-8	0	3	16.1	15.4
-6	0	3	30.8	-30.6
-4	0	3	86.4	-84.1
-2	0	3	57.6	-58.4
0	0	3	120.6	-116.0
2	0	3	40.7	-42.8
4	0	3	24.2	22.6
6	0	3	13.0	13.6
8	0	3	8.0	-8.3
4	12	4	16.3	17.4
2	12	4	34.7	35.8
0	12	4	20.6	22.5
-2	12	4	8.6	8.8
-5	11	4	12.1	-11.7
0	10	4	8.0	-8.7
-4	10	4	10.9	11.2
-6	10	4	8.5	8.6
-5	9	4	24.7	24.6

H	K	L	/FO/	/FC/
3	9	4	18.0	16.8
1	9	4	8.5	9.5
1	9	4	9.8	-10.2
3	9	4	21.4	-22.3
4	9	4	7.6	8.5
7	8	4	10.2	-12.1
4	8	4	11.8	-12.8
1	8	4	15.1	14.0
-1	8	4	12.5	11.7
-2	7	4	8.5	-8.2
-5	7	4	24.7	-23.5
-3	7	4	13.0	-13.0
1	7	4	6.7	7.8
4	6	4	40.1	39.7
2	6	4	94.0	93.5
0	6	4	68.5	65.0
-2	6	4	26.4	24.0
-3	6	4	17.7	18.2
-1	5	4	12.3	-12.4
1	5	4	19.3	-19.5
3	5	4	26.7	-27.4
1	5	4	11.0	-11.0
1	5	4	23.4	24.7
0	5	4	8.8	-9.1
2	4	4	21.8	-22.6
0	4	4	24.5	-25.3
-2	4	4	23.5	24.1
-3	4	4	20.5	20.8
-5	4	4	17.8	16.9
-2	3	4	34.7	34.4
-4	3	4	37.4	35.3
-1	3	4	37.1	37.6
1	3	4	41.8	44.8
1	3	4	51.6	-47.9
3	3	4	40.7	-40.0
5	3	4	18.3	18.7
2	3	4	30.3	29.2
1	2	4	9.0	-9.2
2	2	4	5.6	-5.2
-1	2	4	17.2	-18.3
-3	2	4	34.0	36.0
-4	1	4	23.0	22.5
-2	1	4	14.7	-14.1
-5	1	4	29.2	-29.7
-3	1	4	31.9	-33.7
1	1	4	13.6	-11.5
1	1	4	16.3	15.5
4	1	4	9.8	-9.9
2	1	4	10.5	-11.2
0	0	4	8.5	-8.2

Sample 12. Tas22-1b (continued)

H	K	L	/FO/	/FC/
1	5	11	11.9	-12.7
-1	5	11	16.9	-18.0
-2	4	11	15.6	16.7
0	4	11	23.2	23.5
2	4	11	9.7	9.9
5	3	11	19.1	-20.5
3	3	11	7.5	-8.7
1	3	11	19.7	19.2
-1	3	11	7.1	6.2
-3	3	11	32.4	-32.5
-5	3	11	29.2	-29.4
-7	3	11	17.6	-18.6
-6	2	11	8.1	-8.1
-4	2	11	7.6	7.9
-2	2	11	13.9	14.9
0	2	11	18.1	18.2
2	2	11	20.6	19.9
1	1	11	16.8	-16.4
-1	1	11	17.7	-18.8
-2	0	11	12.9	-13.1
0	0	11	44.6	-45.0
2	0	11	39.8	-38.0
-3	9	12	28.4	28.6
-1	9	12	24.4	22.9
-2	8	12	11.4	11.7
-4	8	12	7.7	8.4
-3	7	12	12.2	-13.2
-1	7	12	7.5	-7.6
2	6	12	32.0	32.1
0	6	12	10.1	8.8
-2	6	12	12.5	-12.3
-5	5	12	7.9	-8.0
-1	5	12	11.3	-11.4
0	4	12	15.3	14.4
-2	4	12	15.2	15.5
-4	4	12	11.9	12.7
-5	3	12	13.4	13.6
-3	3	12	40.7	42.3
-1	3	12	40.4	40.4
3	3	12	16.3	-15.6
-2	2	12	23.5	24.6
-4	2	12	15.7	16.7
-3	1	12	12.5	-14.4
-1	1	12	12.7	-12.9
3	1	12	8.1	8.7
4	0	12	22.5	23.1
2	0	12	41.8	40.7
0	0	12	23.6	22.3
-2	0	12	20.8	-21.0
-6	0	12	22.9	23.1
-1	0	13	23.9	-23.2
-4	0	13	24.7	-25.1
0	0	13	17.4	16.2
-5	0	13	10.6	-11.2
-4	1	13	11.3	12.3
3	3	13	9.2	-9.2
1	3	13	31.8	-30.8
-1	3	13	46.2	-44.3
-3	3	13	10.0	-9.8
-5	3	13	14.5	15.4
-6	4	13	9.4	9.5
-4	4	13	7.7	8.9
-2	4	13	7.9	7.5
2	2	13	7.4	-6.9
1	1	13	8.6	8.3
-3	1	13	7.0	-7.1
-5	1	13	10.5	-11.9
-6	0	13	26.8	-27.4
-4	0	13	27.7	-27.7
0	0	13	24.9	23.9
4	0	13	8.8	-8.9
0	6	14	9.2	9.5
-2	6	14	27.6	26.7
-4	6	14	26.3	25.6
-2	4	14	8.7	-10.0
-3	3	14	17.6	-17.7
1	3	14	8.4	8.9
3	3	14	10.1	9.4
-2	2	14	10.8	-9.0
-4	2	14	7.7	-8.2
3	1	14	8.9	-8.5
2	0	14	6.8	5.5
0	0	14	9.0	9.5
-2	0	14	34.5	33.6
-4	0	14	37.8	38.2
-2	6	15	13.4	-10.7
0	6	15	10.1	-9.6
-3	3	15	10.5	-10.4
0	2	15	11.5	11.3
1	1	15	11.0	-9.7
-1	1	15	9.8	-9.4
-2	0	15	9.6	-9.7
0	0	15	17.9	-17.2
2	0	15	13.6	-14.0
-2	4	16	9.8	9.7
-3	3	16	10.9	10.9
-1	3	16	16.7	15.5
-3	1	16	9.0	-9.2
-1	1	16	8.7	-8.6

Table 8. Observed (FO) and calculated (FC) structure factors for sample 13. Tpq16-6B.

H	K	L	/FO/	/FC/
0	12	0	64.1	66.0
1	11	0	14.7	14.8
6	10	0	9.2	10.4
4	10	0	7.2	8.9
0	10	0	9.1	-8.7
5	9	0	33.4	34.3
3	9	0	33.1	34.0
1	9	0	34.4	-33.3
6	8	0	13.3	13.4
4	8	0	12.7	13.1
0	8	0	8.1	-8.1
7	7	0	7.4	-8.0
5	7	0	11.1	-10.7
3	7	0	7.3	-7.5
1	7	0	30.6	30.8
4	6	0	7.0	5.8
2	6	0	98.9	98.2
0	6	0	171.3	170.6
7	5	0	11.7	-11.1
5	5	0	18.5	-17.4
3	5	0	11.2	11.4
1	5	0	19.7	20.7
8	4	0	6.5	6.4
6	4	0	24.1	22.4
4	4	0	19.5	19.0
0	4	0	32.5	31.1
7	3	0	24.2	23.0
5	3	0	64.8	62.1
3	3	0	52.5	50.8
1	3	0	59.3	-58.3
8	2	0	8.9	8.4
6	2	0	16.7	16.9
4	2	0	33.3	32.4
2	2	0	35.5	34.7
0	2	0	45.7	-45.1
7	1	0	12.1	-12.3
5	1	0	18.8	-19.0
3	1	0	6.6	6.7
1	1	0	41.0	40.0
2	0	0	128.9	127.8
0	0	0	7.0	5.9
3	13	1	8.7	-10.2
-3	13	1	7.5	8.7
2	12	1	37.0	-38.3
4	12	1	17.0	-18.4
5	11	1	8.0	-8.5
3	11	1	16.0	-16.9
-3	11	1	9.0	10.0
-2	10	1	9.5	-9.5
2	10	1	19.1	19.9
4	10	1	15.4	16.2
3	9	1	7.4	6.4
1	9	1	6.8	-6.9
-1	9	1	54.5	-54.3
-3	9	1	78.8	-77.0
-2	8	1	11.9	-12.7
0	8	1	10.8	10.7
2	8	1	29.0	28.2
4	8	1	20.8	20.8
6	8	1	7.6	7.1
5	7	1	17.7	-16.3
3	7	1	33.6	-32.2
-3	7	1	13.6	13.1
-5	7	1	9.6	9.7
-4	6	1	33.4	30.8
-2	6	1	62.2	62.1
0	6	1	54.9	-53.4
2	6	1	88.3	-87.7
4	6	1	36.0	-35.9
6	6	1	17.3	-16.4
5	5	1	15.1	-14.8
3	5	1	31.6	-30.3
1	5	1	41.6	-42.8
-1	5	1	21.7	21.7
-3	5	1	27.8	27.8
-2	4	1	30.8	-31.0
0	4	1	38.5	37.7
2	4	1	58.3	56.0
4	4	1	26.9	25.7
6	4	1	11.4	11.0
7	3	1	9.9	-10.8
5	3	1	18.4	-17.4
1	3	1	43.7	41.7
-1	3	1	132.9	-130.2
-3	3	1	164.8	-163.1
-5	3	1	50.6	-48.0
-4	2	1	17.9	-18.8
-2	2	1	29.4	29.1
0	2	1	8.9	9.8
2	2	1	40.9	42.1
4	2	1	49.0	50.8
6	2	1	8.1	8.1
5	1	1	19.4	-20.4
3	1	1	44.5	-44.1
1	1	1	43.0	-43.1
-1	1	1	18.8	17.1
-3	1	1	28.1	28.1
-8	0	1	25.6	-23.8
-6	0	1	18.0	-17.8
-4	0	1	60.3	58.7
-2	0	1	59.6	57.9
0	0	1	54.5	-55.6
2	0	1	103.2	-103.9
4	0	1	64.1	-64.9
6	0	1	16.7	-16.9
8	0	1	6.3	-5.8
-5	1	1	7.1	6.4
0	14	2	9.8	10.1
-1	13	2	9.7	-9.8
1	13	2	15.4	-16.5
4	12	2	8.5	9.9
-1	11	2	22.0	-23.5
1	11	2	19.4	-19.9
3	11	2	8.0	-8.1
2	10	2	16.9	17.5
0	10	2	23.2	23.3
-2	10	2	8.8	9.3
-3	9	2	18.4	20.5
-1	9	2	72.9	70.8
1	9	2	40.6	38.6
3	9	2	18.4	18.6
5	9	2	11.0	11.3
2	8	2	24.8	24.1
0	8	2	30.5	30.2
-2	8	2	12.6	12.7
-6	8	2	9.1	-9.2
-1	7	2	50.2	-49.2
1	7	2	38.0	-37.1
3	7	2	14.6	-13.7
6	6	2	25.2	23.9
4	6	2	26.9	25.0
2	6	2	19.3	18.7
-4	6	2	52.6	50.7
-6	6	2	58.1	55.4
-3	5	2	15.3	-15.6
-1	5	2	32.0	-31.5
1	5	2	66.6	-65.4
3	5	2	30.7	-29.3
8	4	2	8.8	-8.7
2	4	2	84.1	84.0
0	4	2	37.9	39.2
-2	4	2	13.8	14.2
-6	4	2	13.9	-12.8
-5	3	2	30.6	-29.8
-3	3	2	53.3	51.1
-1	3	2	108.1	105.6
1	3	2	61.3	60.5
3	3	2	38.3	38.2
5	3	2	9.8	8.9
7	3	2	7.5	-7.2
4	2	2	9.9	9.3
2	2	2	10.5	10.7
0	2	2	87.1	88.0
-2	2	2	41.1	42.9
-4	2	2	22.4	-22.0
-6	2	2	9.9	-9.1
-5	1	2	9.7	9.8
-3	1	2	17.7	-17.6
-1	1	2	64.8	-67.8
1	1	2	86.1	-88.6
3	1	2	34.7	-34.8
8	0	2	23.7	25.5
6	0	2	27.6	28.9
4	0	2	24.4	24.7
2	0	2	92.6	92.2
0	0	2	23.3	-22.1
-2	0	2	40.0	-40.6
-4	0	2	92.6	92.5
-6	0	2	68.2	67.3
-7	1	2	7.1	7.0
-7	3	2	19.8	-17.1
-7	5	2	7.5	7.4
-5	5	2	6.9	6.9
-5	7	2	10.1	10.2
-2	14	3	8.6	10.9
-1	13	3	10.8	-12.6
-3	13	3	12.2	-14.6
-4	12	3	29.1	-31.2
-2	12	3	27.3	-29.0
0	12	3	18.5	-19.8
1	11	3	7.4	-7.8
-1	11	3	20.4	-20.9
-3	11	3	14.1	-14.5
-4	10	3	10.8	11.3
-2	10	3	19.3	19.6
0	10	3	8.0	9.0
2	10	3	7.6	-6.9
4	10	3	8.5	-8.5
5	9	3	37.9	-38.4
3	9	3	46.4	-45.0
1	9	3	28.6	-27.0
-1	9	3	20.7	-20.6
-3	9	3	6.2	-6.4
-4	8	3	15.2	15.2
-2	8	3	27.8	27.4
0	8	3	10.3	10.2
4	8	3	11.5	-11.3
3	7	3	12.1	12.1
1	7	3	22.8	-22.1
-1	7	3	47.7	-46.2
-3	7	3	27.5	-26.8
-5	7	3	14.0	-13.4
-6	6	3	18.9	-17.2
-4	6	3	67.1	-65.8
-2	6	3	71.0	-70.2
0	6	3	40.6	-40.4
2	6	3	35.5	-34.4
4	6	3	10.7	9.7
6	6	3	12.9	13.0
5	5	3	7.2	7.1
1	5	3	14.8	-14.0
-1	5	3	47.1	-47.1
-3	5	3	56.5	-55.1
-5	5	3	13.2	-11.7
-4	4	3	25.8	24.8
-2	4	3	49.7	49.4
0	4	3	6.7	-7.0
4	4	3	13.4	-13.0
6	4	3	8.5	-8.1
7	3	3	23.5	-24.0
5	3	3	68.7	-68.1
3	3	3	70.2	-69.0
1	3	3	80.9	-81.4
-1	3	3	93.5	-94.0
-5	3	3	6.6	-5.0
-7	3	3	31.9	-29.1
-8	2	3	6.5	-6.7
-4	2	3	17.8	18.3
-2	2	3	24.4	24.7
0	2	3	58.7	60.1
2	2	3	25.1	-27.0
4	2	3	23.1	-23.0
5	1	3	6.3	6.3
1	1	3	37.6	-38.0
-1	1	3	81.8	-81.7
-3	1	3	65.2	-66.4
-5	1	3	17.1	-17.0
-8	0	3	12.5	11.7
-6	0	3	30.6	-29.4
-4	0	3	82.1	-84.1
-2	0	3	60.1	-60.0
0	0	3	117.2	-118.7
2	0	3	41.5	-43.0
4	0	3	19.0	19.4
6	0	3	10.3	10.5
2	4	3	5.9	-6.0
1	13	4	7.8	8.7
4	12	4	20.2	21.5
2	12	4	41.1	43.4
0	12	4	28.2	29.2
-2	12	4	11.7	12.7
-5	11	4	11.9	-13.4
-3	11	4	8.0	-8.2
2	10	4	10.1	-10.1
0	10	4	9.0	-9.7
-4	10	4	11.9	12.7
-6	10	4	8.6	8.8
-5	9	4	27.6	26.5
-3	9	4	20.9	20.1
-1	9	4	10.6	10.9
1	9	4	10.7	-9.9
3	9	4	21.7	-22.2
5	9	4	9.7	10.0
2	8	4	13.1	-12.8
0	8	4	14.5	-14.5
-2	8	4	5.8	5.7
-4	8	4	15.0	14.6
-6	8	4	12.7	11.3
-7	7	4	7.9	-7.2
-5	7	4	24.2	-23.6
-3	7	4	14.5	-14.5
-1	7	4	7.5	8.1
3	7	4	7.8	7.2
4	6	4	43.0	41.9
2	6	4	101.8	99.8
0	6	4	74.2	73.2
-2	6	4	27.7	26.7
-4	6	4	19.8	19.0
-7	5	4	11.3	-11.0
-5	5	4	19.8	-19.6
-3	5	4	29.0	-27.6
-1	5	4	11.3	-11.2
1	5	4	24.4	25.4
5	5	4	9.2	-8.9
4	4	4	6.8	5.9
2	4	4	23.4	-23.2
0	4	4	25.4	-26.6
-2	4	4	24.3	24.4
-4	4	4	20.2	19.7
-6	4	4	16.3	15.4
-7	3	4	32.9	31.0
-5	3	4	36.4	35.3
-3	3	4	38.3	39.3
-1	3	4	45.0	45.6
1	3	4	46.8	-46.9
3	3	4	38.5	-37.8
5	3	4	18.6	18.8
7	3	4	26.5	27.5
6	2	4	9.6	10.7
4	2	4	9.2	-8.7

Sample 13. Tpq16-6B (continued)

H	K	L	/FO/	/FC/
0	0	9	13.5	-13.6
4	0	9	12.3	-12.3
6	0	9	21.7	-22.7
5	5	9	7.5	-8.1
-4	10	10	7.0	-7.0
1	9	10	13.6	13.4
3	9	10	22.6	22.9
4	8	10	8.1	7.4
-4	8	10	8.0	-8.7
-3	7	10	8.6	8.4
1	7	10	13.6	-14.8
3	7	10	9.2	-10.1
4	6	10	11.7	-10.9
0	6	10	33.8	31.9
-2	6	10	35.4	34.2
-4	6	10	33.3	33.1
-6	6	10	22.1	22.8
-5	5	10	8.0	8.2
-3	5	10	5.9	6.4
-1	5	10	7.7	-7.2
1	5	10	9.4	-9.2
3	5	10	12.8	-13.8
5	5	10	8.2	-7.4
4	4	10	12.6	12.0
2	4	10	11.5	11.5
-4	4	10	13.0	-13.6
-5	3	10	8.9	-8.5
1	3	10	13.4	13.0
3	3	10	37.6	36.3
5	3	10	19.2	19.8
4	2	10	7.4	7.9
2	2	10	19.1	19.2
0	2	10	12.2	11.7
-2	2	10	14.3	-15.1
-4	2	10	7.2	-7.4
-5	1	10	6.8	7.2
-3	1	10	7.6	8.6
1	1	10	15.7	-15.4
3	1	10	15.7	-16.0
5	1	10	7.6	-7.9
4	0	10	8.4	-8.4
0	0	10	38.5	37.9
-2	0	10	60.2	60.2
-4	0	10	36.6	37.1
-6	0	10	26.4	27.3
0	4	10	6.5	5.7
2	8	10	8.8	9.3
2	10	10	7.2	6.7
0	10	11	10.8	10.5
1	9	11	12.5	12.2

H	K	L	/FO/	/FC/
-3	9	11	15.6	-16.4
-2	8	11	10.0	10.1
0	8	11	13.4	13.9
1	7	11	11.6	-11.9
-1	7	11	7.3	-7.4
-3	7	11	6.8	-6.7
-2	6	11	13.8	-13.8
0	6	11	41.2	-39.6
2	6	11	23.3	-24.0
1	5	11	12.9	-12.6
-1	5	11	17.7	-17.8
-2	4	11	15.5	15.8
0	4	11	23.5	23.1
2	4	11	10.1	10.2
5	3	11	19.6	-19.8
3	3	11	9.4	-8.9
1	3	11	18.6	16.7
-3	3	11	32.6	-31.6
-5	3	11	27.5	-26.9
-7	3	11	14.6	-15.8
-6	2	11	7.2	-7.3
-4	2	11	7.4	7.2
-2	2	11	13.7	13.8
0	2	11	18.3	17.7
2	2	11	21.4	19.9
1	1	11	16.3	-16.8
-1	1	11	18.1	-18.0
-2	0	11	13.7	-13.7
0	0	11	44.2	-43.4
2	0	11	37.4	-37.3
2	8	11	8.5	8.8
-2	10	12	8.0	8.8
3	9	12	28.6	29.0
-1	9	12	23.7	24.4
0	8	12	8.0	7.9
-2	8	12	11.3	11.5
-4	8	12	7.4	8.1
-3	7	12	12.1	-12.3
-1	7	12	7.2	-7.7
2	6	12	33.2	33.1
0	6	12	9.6	9.6
-2	6	12	10.2	-9.5
-5	5	12	7.0	-6.9
-3	5	12	7.8	-8.6
-1	5	12	11.4	-10.9
0	4	12	16.1	15.3
-2	4	12	15.7	14.9
-4	4	12	11.6	11.6
-5	3	12	13.4	12.8
-3	3	12	41.0	39.4

H	K	L	/FO/	/FC/
-1	3	12	41.8	39.6
3	3	12	14.1	-13.8
0	2	12	7.7	6.9
-2	2	12	24.6	23.7
-4	2	12	13.9	14.8
-3	1	12	12.5	-12.7
-1	1	12	13.2	-12.2
3	1	12	8.1	8.2
4	0	12	22.4	23.1
2	0	12	40.9	40.0
0	0	12	23.3	22.6
-2	0	12	19.2	-17.3
-6	0	12	20.0	20.3
3	5	12	7.4	8.3
-1	9	13	23.1	-24.1
1	7	13	7.0	8.7
-4	6	13	23.1	-23.7
0	6	13	15.3	14.9
-5	5	13	9.1	-9.5
-4	4	13	11.1	11.3
3	3	13	9.9	-9.8
1	3	13	33.0	-30.8
-1	3	13	44.1	-42.1
-3	3	13	10.7	-9.4
-5	3	13	12.8	11.9
-2	2	13	8.3	7.6
0	2	13	8.1	-7.8
1	1	13	8.0	7.7
-3	1	13	6.8	-6.8
-5	1	13	10.1	-9.9
-6	0	13	22.7	-22.8
-4	0	13	24.2	-24.7
0	0	13	24.3	21.8
4	0	13	9.4	-9.0
-6	2	13	6.9	7.6
-4	2	13	6.2	7.8
-1	5	13	6.2	6.3
0	6	14	11.4	10.7
-2	6	14	26.3	26.4
-4	6	14	22.7	23.4
2	4	14	7.3	7.0
-2	4	14	9.1	-8.9
-3	3	14	16.0	-14.7
1	3	14	9.8	8.9
-2	2	14	8.3	-7.8
-4	2	14	6.8	-6.6
3	1	14	7.5	-8.4
2	0	14	7.0	6.0
0	0	14	11.0	10.1
-2	0	14	31.7	31.8

H	K	L	/FO/	/FC/
-4	0	14	35.1	33.6
-1	5	14	6.8	5.9
-2	6	15	10.9	-10.8
-1	5	15	7.8	-7.4
-1	3	15	7.3	-6.4
-3	3	15	11.8	-10.6

H	K	L	/FO/	/FC/
0	2	15	10.8	10.5
1	1	15	9.9	-9.6
-1	1	15	9.8	-9.2
-2	0	15	10.7	-9.3
0	0	15	18.0	-16.8

H	K	L	/FO/	/FC/
2	0	15	13.7	-13.1
-1	3	16	14.5	14.0
-3	1	16	8.0	-8.0
-1	1	16	7.3	-7.8
-3	3	16	9.9	9.9