

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
3	1	-16	9.1	-9.9	1	9	-11	20.3	20.0	2	8	-9	8.2	-7.3
1	3	-16	11.3	11.6	3	9	-12	26.9	26.9	6	7	-9	13.0	-12.8
2	6	-15	13.3	-13.5	0	10	-11	8.0	8.7	6	6	-9	20.6	-21.0
0	2	-15	11.5	12.5	3	9	-11	12.9	-11.7	7	5	-9	8.5	-10.2
1	1	-15	10.5	-11.8	-1	9	-11	10.9	10.8	0	5	-9	9.6	-9.5
-1	1	-15	9.9	-9.2	0	8	-11	12.9	13.9	0	4	-9	23.0	-22.8
0	6	-15	10.1	-17.4	2	0	-11	11.1	10.6	2	4	-9	8.3	-7.6
2	6	-15	10.1	-10.1	3	7	-11	8.6	-8.2	0	3	-9	24.5	-23.8
4	0	-14	36.0	38.1	0	0	-11	35.2	-34.8	3	3	-9	59.0	-57.9
2	0	-14	28.8	30.0	2	0	-11	13.0	-11.0	1	3	-9	62.0	-61.9
4	2	-14	8.6	-8.9	1	0	-11	16.0	-16.3	-1	3	-9	52.4	-51.4
-1	3	-14	9.7	9.7	-1	0	-11	0.0	-9.4	2	2	-9	25.0	-24.9
3	3	-14	16.9	-16.5	0	4	-11	23.5	24.0	6	2	-9	16.3	16.9
4	6	-14	22.1	22.9	2	4	-11	16.8	17.5	7	1	-9	11.9	-13.2
2	6	-14	23.3	23.5	7	3	-11	14.0	-15.5	0	1	-9	14.5	-15.2
1	9	-13	20.8	-20.8	5	3	-11	25.1	-24.8	0	0	-9	21.0	-21.4
-1	7	-13	8.7	8.0	3	3	-11	30.5	-29.5	2	0	-9	16.6	16.3
0	6	-13	13.5	14.8	-1	3	-11	13.8	14.4	0	0	-9	36.7	-36.7
2	6	-13	9.9	9.6	0	2	-11	16.0	15.7	J	1	-9	6.0	-5.5
4	6	-13	22.8	-21.9	2	2	-11	16.0	16.0	1	1	-9	15.0	-14.6
5	5	-13	9.0	-9.1	4	2	-11	12.3	12.0	J	1	-8	33.3	-33.5
4	4	-13	13.5	13.4	3	1	-11	7.0	-7.1	0	1	-8	21.1	-21.4
5	3	-13	11.8	13.3	1	1	-11	17.5	-17.1	0	0	-8	18.2	10.1
3	3	-13	11.4	-11.1	-1	1	-11	13.1	-13.0	0	0	-8	10.0	-11.9
1	3	-13	42.5	-42.7	0	1	-11	36.0	-35.9	4	0	-8	9.0	-9.7
-1	3	-13	26.1	-27.2	2	0	-11	12.2	-11.8	2	0	-8	33.3	32.9
2	2	-13	10.6	10.2	-1	1	-10	16.3	-16.0	0	0	-8	63.0	63.2
6	2	-13	8.6	9.2	1	1	-10	10.3	-10.0	6	2	-8	15.8	15.1
0	0	-13	21.1	22.9	6	0	-10	28.7	29.4	4	2	-8	14.2	14.2
4	0	-13	20.9	-19.8	4	0	-10	31.9	31.6	2	2	-8	23.2	23.5
6	0	-13	22.5	-23.3	2	0	-10	56.1	55.6	-1	3	-8	14.5	-14.9
5	1	-13	8.9	-9.2	0	0	-10	36.0	34.3	1	3	-8	16.3	-16.8
1	1	-12	10.4	-10.4	2	2	-10	14.7	-15.0	J	3	-8	49.0	49.5
3	1	-12	11.3	-11.6	0	2	-10	13.8	13.7	0	3	-8	55.5	54.3
6	0	-12	21.9	22.9	-1	3	-10	10.9	10.9	4	4	-8	30.9	29.9
2	0	-12	10.4	-10.1	5	3	-10	11.6	-11.7	2	4	-8	14.2	13.5
0	0	-12	20.5	27.0	4	4	-10	10.0	-10.0	0	4	-8	13.2	-13.2
4	2	-12	16.1	16.2	1	0	-10	10.4	-10.6	J	0	-8	30.3	-29.8
2	2	-12	20.1	20.4	0	0	-10	22.0	22.7	0	0	-8	18.1	-18.2
1	3	-12	35.5	35.3	4	0	-10	31.1	31.0	4	0	-8	31.2	-31.8
J	3	-12	39.2	37.9	2	6	-10	27.3	25.0	0	0	-8	26.6	25.1
5	3	-12	13.7	14.3	0	6	-10	27.6	27.6	0	6	-8	55.1	54.3
4	4	-12	13.6	13.4	-1	7	-10	13.5	-15.0	1	7	-8	14.6	-14.8
2	4	-12	13.6	12.7	-1	9	-10	11.5	11.9	1	7	-8	14.6	-14.8
0	4	-12	16.2	15.9	-1	11	-10	8.0	-8.0	1	7	-8	11.1	-12.4
1	5	-12	9.1	-9.2	5	9	-9	9.0	-9.2	0	8	-8	18.4	15.8
0	6	-12	9.6	9.9	3	9	-8	38.4	-38.0	0	8	-8	9.6	8.2
J	7	-12	11.5	-11.5	1	9	-8	29.6	-28.9	0	8	-8	7.3	-7.1
4	6	-12	8.4	8.2	-1	9	-8	21.0	-21.1	-1	9	-8	9.7	-9.8
2	6	-12	9.2	9.4	0	8	-8	11.5	-11.4	1	9	-8	24.3	22.6
5	9	-8	29.2	30.3	0	2	-6	10.1	-10.6	1	1	-5	10.4	9.0
4	10	-8	10.7	9.6	2	2	-6	31.6	33.5	0	0	-5	94.3	93.0
1	11	-8	7.3	-8.0	0	2	-6	20.1	20.5	2	0	-5	37.2	36.7
3	11	-8	8.9	-8.5	-1	3	-6	112.8	110.7	4	0	-5	36.1	-36.9
0	12	-8	19.5	19.8	1	3	-6	46.8	48.3	0	0	-5	13.0	-12.7
0	12	-7	17.9	-18.2	3	3	-6	32.3	-33.5	0	0	-5	14.0	-14.7
2	12	-7	28.2	-28.5	7	3	-6	11.2	11.5	-1	1	-4	7.4	7.4
1	11	-7	13.3	-13.5	0	4	-6	54.7	54.9	1	1	-4	17.0	-16.8
0	10	-7	13.0	13.3	-1	5	-6	29.3	-28.7	J	1	-4	32.4	-32.9
2	10	-7	15.7	16.6	1	5	-6	10.2	-10.2	0	1	-4	29.0	-28.5
5	9	-7	26.5	-25.8	3	5	-6	18.2	17.8	7	1	-4	13.2	-13.5
1	9	-7	19.4	20.1	5	5	-6	6.5	8.3	4	0	-4	18.7	18.2
-1	9	-7	21.6	-20.9	6	6	-6	22.1	22.2	2	0	-4	76.7	78.8
0	8	-7	22.9	23.1	4	6	-6	68.7	68.6	0	0	-4	50.9	52.9
2	8	-7	18.6	18.2	2	6	-6	75.3	73.8	0	2	-4	18.6	17.7
4	8	-7	10.1	10.3	-1	7	-6	11.8	-12.4	4	2	-4	32.6	33.0
3	7	-7	15.4	-14.9	5	7	-6	14.3	13.5	2	2	-4	22.8	-23.7
1	7	-7	26.5	-26.3	0	8	-6	24.1	24.1	-1	3	-4	35.1	-34.7
0	6	-7	47.1	-47.1	-1	9	-6	48.0	48.7	1	3	-4	39.9	43.4
2	6	-7	59.8	-59.9	1	9	-6	20.4	20.1	3	3	-4	27.5	28.0
4	6	-7	22.2	-20.6	0	10	-6	13.7	13.8	0	3	-4	28.5	27.6
6	6	-7	14.0	15.1	4	12	-6	27.4	27.6	7	3	-4	28.6	30.3
J	5	-7	13.7	-13.2	2	12	-6	25.9	24.8	8	4	-4	13.2	13.4
1	5	-7	23.0	-22.6	0	12	-6	12.0	13.3	4	4	-4	13.0	12.7
-1	5	-7	23.8	-24.2	1	11	-6	13.6	13.1	2	4	-4	24.5	24.9
6	4	-7	46.3	39.4	5	9	-6	10.2	-9.8	0	4	-4	21.4	-22.0
2	4	-7	21.8	21.5	J	9	-6	26.3	-25.8	-1	0	-4	18.2	18.5
4	4	-7	19.9	19.6	1	9	-6	64.5	-64.9	1	5	-4	13.8	-13.8
7	3	-7	35.1	-35.8	-1	9	-6	35.4	-35.3	3	5	-4	26.8	-28.5
3	3	-7	39.0	-38.5	1	7	-6	21.7	21.4	5	5	-4	18.8	-18.8
J	3	-7	8.4	8.3	0	6	-6	31.8	32.2	7	6	-4	10.4	-12.5
1	3	-7	21.2	21.9	2	6	-6	15.1	15.8	4	6	-4	22.8	21.4
-1	3	-7	32.0	-31.5	4	6	-6	8.1	-7.6	0	8	-4	21.0	20.3
0	2	-7	33.9	33.6	6	6	-6	17.3	-18.5	0	8	-4	61.8	61.4
2	2	-7	57.5	58.7	7	5	-6	10.5	-10.9	J	7	-4	12.6	-13.1
J	1	-7	20.4	-20.2	3	0	-6	18.9	18.8	5	7	-4	24.3	-23.2
1	1	-7	35.9	-36.6	-1	5	-6	5.2	5.3	0	8	-4	10.0	8.9
-1	1	-7	26.3	-25.7	0	4	-6	16.2	16.3	4	8	-4	8.9	8.9
0	0	-7	51.7	-51.9	4	4	-6	12.3	-11.8	0	8	-4	14.1	-13.2
2	0	-7	114.8	-115.9	6	4	-6	13.2	12.6	1	9	-4	8.1	7.4
4	0	-7	12.6	-12.9	5	3	-6	26.0	-24.6	3	9	-4	12.9	13.3
6	0	-7	20.2	-21.8	3	3	-6	62.9	-63.5	5	9	-4	22.3	21.5
-1	1	-6	30.5	-30.2	1	3	-6	113.4	-115.2	4	10	-4	10.4	9.8
1	1	-6	8.5	-8.6	-1	3	-6	91.0	-90.7	5	11	-4	12.0	-13.0
J	1	-6	15.0	15.3	0	0	-6	8.7	-8.4	2	12	-4	8.5	9.5
5	1	-6	13.7	13.5	2	2	-6	12.5	-13.3	0	12	-4	26.0	26.0
4	0	-6	43.3	42.5	4	2	-6	14.8	13.7	J	3	-3	13.0	-12.8
4	0	-6	93.8	93.3	8	2	-6	7.6	8.8	1	3	-3	8.8	-9.1
2	0	-6	91.7	94.2	7	1	-6	11.4	-11.6	0	12	-3	15.8	-15.5

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-1	1	-1	41.7	-45.1	-1	7	2	48.1	-49.6	-1	9	-3	36.3	-29.8
-1	1	1	14.4	12.9	-1	7	3	48.1	-47.7	-1	9	-2	32.5	32.7
-1	1	2	67.9	-68.9	-1	7	4	7.6	7.2	-1	7	-14	8.6	-8.2
-1	1	3	82.6	-88.1	-1	7	5	25.8	25.3	-1	7	-13	12.9	14.0
-1	1	4	19.5	-19.6	-1	7	7	35.5	-35.6	-1	7	-12	6.6	6.6
-1	1	5	11.8	9.7	-1	7	8	19.6	-19.4	-1	7	-11	13.5	-15.0
-1	1	6	9.2	-10.2	-1	7	11	8.1	-8.2	-1	7	-10	21.0	-21.7
-1	1	7	41.0	-48.7	-1	7	12	7.5	-7.9	-1	7	-9	8.0	-8.0
-1	1	8	16.7	-17.2	-1	8	1	8.1	-7.4	-1	7	-8	6.7	6.9
-1	1	10	12.4	-12.2	-1	8	0	30.8	-31.9	-1	7	-7	8.2	-8.5
-1	1	11	22.8	-22.5	-1	8	1	50.8	-50.6	-1	7	-6	16.1	-14.7
-1	1	12	14.5	-13.9	-1	8	2	73.0	72.9	-1	7	-5	4.7	-4.2
-1	1	13	7.6	7.2	-1	8	3	26.4	-27.0	-1	7	-3	25.4	-25.6
-1	1	15	19.5	-18.5	-1	8	1	9.3	9.5	-1	7	-2	35.2	-35.8
-1	1	16	13.5	-13.3	-1	8	6	85.2	-84.5	-1	5	-14	11.8	-11.6
-1	1	0	32.4	35.4	-1	8	4	27.2	26.8	-1	5	-13	5.7	6.2
-1	1	9	5.1	4.9	-1	8	7	27.2	27.3	-1	5	-11	13.3	-14.1
-1	3	-1	48.2	35.9	-1	9	9	42.2	-42.6	-1	5	-10	11.9	-13.0
-1	3	0	53.3	-50.9	-1	9	12	33.9	34.4	-1	5	-7	30.3	-30.1
-1	3	1	110.9	-119.2	-1	9	13	37.5	-37.4	-1	5	-6	34.3	-34.1
-1	3	2	97.6	96.2	-1	11	0	17.8	17.9	-1	5	-4	21.6	20.7
-1	3	3	107.5	-109.0	-1	11	2	28.3	-28.6	-1	5	-3	15.4	-15.6
-1	3	4	45.3	46.2	-1	11	3	24.1	-24.2	-1	5	-2	64.5	-65.3
-1	3	5	130.2	-128.7	-1	11	4	5.3	5.0	-1	3	-15	13.0	-11.8
-1	3	6	54.2	53.5	-1	11	5	18.9	18.9	-1	3	-14	18.4	17.7
-1	3	7	25.0	24.0	-1	11	7	20.7	-20.5	-1	3	-13	46.4	-45.2
-1	3	8	18.3	-20.3	-1	11	8	12.1	-11.9	-1	3	-11	21.1	21.0
-1	3	9	74.7	-75.6	-1	13	-1	11.9	-12.6	-1	3	-10	15.1	15.1
-1	3	12	58.5	58.6	-1	13	0	11.1	10.8	-1	3	-9	68.1	-67.6
-1	3	13	65.6	-64.4	-1	13	1	8.7	8.5	-1	3	-8	18.4	-18.2
-1	3	14	5.8	-5.9	-1	13	2	8.5	-8.5	-1	3	-7	37.3	-39.1
-1	3	15	10.1	-9.7	-1	13	3	14.7	-14.7	-1	3	-6	131.6	131.1
-1	3	16	28.5	21.8	-1	13	7	11.0	-10.4	-1	3	-5	104.1	-104.3
-1	5	-1	39.3	-48.2	-1	13	7	12.3	-11.5	-1	3	-4	48.6	-38.2
-1	5	0	15.4	15.9	-1	13	-6	11.3	-11.8	-1	3	-3	88.2	-84.9
-1	5	1	20.2	19.4	-1	13	-4	13.2	12.6	-1	3	-2	42.7	41.6
-1	5	2	36.8	-31.5	-1	13	-2	20.2	-19.3	-1	1	-15	17.6	-17.5
-1	5	3	48.4	-46.6	-1	11	-10	14.4	-14.6	-1	1	-14	13.0	-12.9
-1	5	4	15.4	-15.4	-1	11	-8	10.5	-10.3	-1	1	-13	9.3	9.6
-1	5	8	12.3	-12.3	-1	11	-3	10.7	-10.7	-1	1	-11	19.7	-18.7
-1	5	7	27.1	-28.0	-1	11	-2	21.3	-21.0	-1	1	-10	28.8	-31.3
-1	5	0	8.1	-8.0	-1	10	-12	6.6	-7.1	-1	1	-7	29.0	-30.8
-1	5	9	8.7	8.8	-1	10	-11	16.8	16.9	-1	1	-6	34.8	-34.1
-1	5	10	13.0	-13.0	-1	10	-10	19.6	19.7	-1	1	-4	8.4	8.8
-1	5	11	21.7	-22.8	-1	10	-9	33.9	-33.1	-1	1	-3	40.9	-41.2
-1	5	12	12.5	-12.6	-1	10	-8	14.3	-14.4	-1	1	-2	98.0	-86.9
-1	5	13	10.1	10.7	-1	10	-7	31.1	-30.5	-1	1	-1	5.2	-5.0
-1	5	14	7.6	7.0	-1	10	-6	68.8	67.8	0	14	4	8.8	-8.9
-1	5	15	15.1	-15.4	-1	10	-5	47.2	-47.2	0	14	2	10.1	10.1
1	7	8	29.3	30.4	-1	10	-4	7.2	-6.9	0	12	8	33.2	33.2

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	12	7	30.8	-29.6	0	4	8	63.8	62.9	2	10	6	27.6	26.3
0	12	5	20.8	20.1	0	4	0	18.5	18.9	2	10	5	12.3	11.8
0	12	4	38.2	29.7	0	4	4	23.9	-23.2	2	10	4	9.5	-9.4
0	12	3	23.7	-22.9	0	4	3	14.8	-15.5	2	10	3	10.8	-11.2
0	12	1	20.8	-21.5	0	4	2	29.7	31.3	2	10	2	14.2	14.5
0	12	0	73.4	73.7	0	4	1	42.0	43.6	2	10	1	18.8	20.0
0	10	12	7.6	7.6	0	4	0	44.5	44.8	2	10	-1	5.7	-6.3
0	10	11	14.4	14.5	0	2	10	8.2	8.0	2	8	11	11.1	11.6
0	10	10	7.6	7.1	0	2	10	20.0	20.3	2	8	10	11.4	11.9
0	10	9	11.3	-10.7	0	2	13	10.9	-10.6	2	8	8	11.2	-11.4
0	10	7	18.2	18.8	0	2	12	7.5	6.9	2	8	7	9.2	9.6
0	10	6	20.2	19.4	0	2	11	21.4	21.6	2	8	6	28.9	27.2
0	10	4	8.9	-9.0	0	2	10	17.8	18.0	2	8	5	11.3	10.8
0	10	3	7.9	8.3	0	2	8	4.5	5.0	2	8	4	16.1	-14.8
0	10	2	23.9	24.2	0	2	7	38.7	38.7	2	8	3	4.7	-5.4
0	10	1	4.9	4.5	0	2	6	23.5	23.5	2	8	2	24.7	25.5
0	10	0	7.1	-7.9	0	2	5	9.8	-7.8	2	8	1	38.5	38.7
0	8	13	6.5	-6.2	0	2	3	64.1	60.9	2	8	0	10.9	-12.2
0	8	12	13.3	13.5	0	2	2	85.5	84.4	2	8	-1	55.8	56.1
0	8	11	20.7	21.7	0	2	1	11.8	14.9	2	8	-2	28.0	-28.7
0	8	10	6.1	5.7	0	2	0	38.1	-39.7	2	6	9	7.1	-7.4
0	8	9	18.3	-18.9	0	0	10	20.4	-20.9	2	6	8	39.5	39.2
0	8	8	9.9	-9.9	0	0	13	34.7	34.4	2	6	7	9.9	-10.6
0	8	7	30.3	38.8	0	0	12	40.9	39.7	2	6	6	14.9	-14.8
0	8	6	31.0	31.0	0	0	11	68.8	-49.3	2	6	4	105.0	105.9
0	8	4	17.2	-16.6	0	0	10	47.1	45.3	2	6	3	46.4	-42.1
0	8	3	5.1	4.3	0	0	9	24.9	-26.9	2	6	2	28.9	21.1
0	8	2	25.2	25.2	0	0	8	73.2	75.7	2	6	1	87.5	-87.6
0	8	1	15.2	15.2	0	0	7	58.8	-58.4	2	6	0	98.6	109.9
0	6	14	12.5	12.7	0	0	6	48.4	48.4	2	6	-1	86.3	65.8
0	6	13	23.7	24.4	0	0	5	105.0	103.1	2	4	14	14.8	15.2
0	6	12	16.1	16.1	0	0	4	58.0	57.5	2	4	11	11.2	11.7
0	6	11	49.7	-51.8	0	0	3	187.0	-189.4	2	4	10	14.8	14.8
0	6	10	39.3	39.2	0	0	2	15.9	-15.0	2	4	8	5.8	-6.5
0	6	8	70.1	70.3	0	0	1	50.4	-48.9	2	4	7	18.0	18.2
0	6	7	58.4	-58.0	0	0	0	5.7	-4.7	2	4	6	40.1	39.5
0	6	6	8.8	-8.7	2	14	-9	8.7	8.4	2	4	5	7.8	7.6
0	6	5	38.4	37.7	2	14	1	13.2	13.1	2	4	4	22.8	-20.2
0	6	4	70.3	70.1	2	14	-1	6.2	-6.5	2	4	2	55.7	54.9
0	6	3	28.8	-30.8	2	12	8	23.2	22.6	2	4	1	56.2	56.2
0	6	2	11.2	13.4	2	12	6	11.5	-13.1	2	4	-1	26.7	-27.4
0	4	15	6.5	6.3	2	12	5	14.2	-13.9	2	2	13	10.5	-10.4
0	4	13	6.8	-6.7	2	12	4	50.5	49.6	2	2	11	39.3	31.1
0	4	12	23.3	23.8	2	12	3	15.9	-15.9	2	2	10	27.2	28.2
0	4	11	31.8	33.2	2	12	2	10.9	10.5	2	2	8	33.3	-33.5
0	4	10	9.1	9.4	2	12	1	43.7	-42.4	2	2	6	59.2	69.0
0	4	9	28.5	-29.8	2	12	0	39.9	40.8	2	2	5	58.4	51.7
0	4	8	15.8	-15.3	2	12	-1	23.6	24.3	2	2	3	26.3	-26.6
0	4	7	47.3	48.3	2	10	10	10.7	11.1	2	2	1	39.2	39.3
					2	10	8	13.2	-13.4	2	2	0	45.0	44.8

Sample 2. Tas27-2Bb (continued)

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
4	0	-6	188.1	187.1	4	10	-4	14.5	14.6	5	9	2	17.2	16.8
4	0	-7	15.8	-15.0	4	10	-7	5.6	5.8	5	9	3	49.9	-49.6
4	0	-8	10.1	-10.5	4	10	-8	15.3	14.5	5	9	4	13.8	14.0
4	0	-10	38.5	39.4	4	10	-10	8.0	-8.4	5	9	5	11.9	12.7
4	0	-11	7.5	-7.8	4	12	-2	29.2	28.4	5	9	7	21.5	-22.8
4	0	-13	28.8	-28.7	4	12	-3	40.5	-40.8	5	11	-1	12.3	12.2
4	0	-14	57.2	57.1	4	12	-4	9.2	8.6	5	11	1	11.8	-11.8
4	2	-2	23.3	-24.4	4	12	-5	10.7	-10.3	5	11	-7	7.6	7.3
4	2	-3	16.9	17.7	4	12	-6	44.4	44.7	5	11	-8	12.4	12.9
4	2	-4	36.1	37.8	4	12	-7	12.5	-12.6	5	11	-4	20.3	-20.8
4	2	-5	16.0	15.9	5	1	-1	7.9	7.6	5	11	-3	10.9	-11.7
4	2	-7	8.1	7.4	5	1	0	21.6	-20.8	5	11	-2	9.1	8.6
4	2	-8	15.7	16.4	5	1	1	24.2	-24.1	5	9	-9	15.3	-14.0
4	2	-10	5.4	-6.2	5	1	3	6.0	5.7	5	9	-8	45.8	45.5
4	2	-11	16.5	15.2	5	1	4	12.2	-11.6	5	9	-7	39.3	-38.4
4	2	-12	23.7	22.1	5	1	5	23.1	-22.9	5	9	-6	10.1	-10.4
4	3	-13	8.4	8.7	5	1	7	11.5	12.0	5	9	-5	14.6	-14.2
4	2	-14	13.4	-13.5	5	1	8	5.4	-5.5	5	9	-4	32.0	31.9
4	2	-15	7.2	-8.6	5	1	9	16.1	-16.5	5	9	-2	24.8	-24.1
4	4	-2	8.4	8.6	5	1	10	12.4	-11.4	5	7	-9	28.3	-18.3
4	4	-3	24.6	24.2	5	1	11	6.4	6.6	5	7	-8	15.8	-16.4
4	4	-4	14.5	14.6	5	1	11	52.0	-51.3	5	7	-7	7.1	7.6
4	4	-5	13.2	-14.0	5	1	0	73.8	73.3	5	7	-6	19.1	18.9
4	4	-7	23.2	23.6	5	1	1	26.8	-26.8	5	7	-5	5.8	-5.3
4	4	-8	36.1	36.6	5	1	2	9.0	9.6	5	7	-4	29.2	-30.6
4	4	-10	19.9	-20.2	5	1	3	81.7	-84.4	5	7	-3	19.4	-19.4
4	4	-12	19.8	19.0	5	1	4	26.4	27.0	5	7	-2	13.3	13.0
4	4	-13	19.5	19.3	5	1	5	27.0	26.8	5	5	-13	13.9	-14.3
4	4	-15	7.4	-8.0	5	1	7	42.8	-42.2	5	5	-12	10.8	-11.1
4	6	-2	50.4	50.7	5	1	8	6.0	-5.8	5	5	-10	11.1	11.3
4	6	-3	73.0	-73.2	5	1	10	35.3	34.1	5	5	-9	12.0	-12.0
4	6	-4	27.3	27.0	5	1	11	38.7	-37.3	5	5	-8	23.6	-23.6
4	6	-5	9.3	-9.5	5	1	0	20.8	-20.6	5	5	-6	10.9	10.6
4	6	-6	86.7	85.1	5	0	1	15.7	-16.8	5	5	-4	22.5	-22.8
4	6	-7	27.5	-27.2	5	0	2	5.7	5.8	5	5	-3	13.0	-13.3
4	6	-8	26.4	-27.4	5	0	3	8.2	8.7	5	5	-2	6.0	6.7
4	6	-10	41.3	42.4	5	0	4	11.1	-12.3	5	3	-14	6.4	-7.2
4	6	-11	5.7	6.4	5	0	5	22.1	-22.9	5	3	-13	19.0	19.3
4	6	-13	33.8	-34.7	5	0	7	13.4	13.6	5	3	-12	20.2	20.6
4	6	-14	38.8	37.8	5	0	9	13.0	-12.0	5	3	-11	33.9	-33.7
4	8	-3	17.3	16.0	5	0	10	12.1	-12.1	5	3	-10	14.8	-14.6
4	8	-4	11.9	11.5	5	7	-1	14.8	14.8	5	3	-9	30.4	-31.0
4	8	-5	6.0	-5.8	5	7	0	6.9	-9.8	5	3	-8	87.1	88.0
4	8	-6	5.3	-5.8	5	7	1	21.1	-20.9	5	3	-7	45.8	-47.3
4	8	-7	13.9	14.1	5	7	2	10.0	-10.3	5	3	-6	6.7	-6.9
4	8	-8	22.3	21.7	5	7	8	9.0	-8.5	5	3	-5	31.4	-30.2
4	8	-10	13.8	-14.8	5	7	5	12.8	-13.8	5	3	-4	34.1	33.4
4	8	-12	13.8	13.6	5	9	-1	39.9	-40.4	5	3	-3	8.0	-7.8
4	10	-2	5.7	-6.0	5	9	0	41.7	42.6	5	3	-2	32.4	-31.5
4	10	-3	11.5	11.0	5	9	1	11.3	-10.4	5	1	-13	14.5	-13.8

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
5	1	-12	9.6	-9.7	6	0	-3	42.6	-43.0	7	3	5	14.9	-13.8
5	1	-10	8.6	8.3	6	0	-4	6.3	-6.8	7	5	0	15.5	-16.1
5	1	-9	18.5	-18.6	6	0	-5	16.3	-16.0	7	5	4	8.8	-9.4
5	1	-8	20.1	-26.0	6	0	-6	55.4	54.6	7	7	-1	7.8	-7.3
5	1	-6	16.7	16.1	6	0	-7	25.2	26.4	7	7	0	9.5	-9.7
5	1	-5	4.7	-4.1	6	0	-8	14.4	-15.3	7	7	2	7.6	8.1
5	1	-4	33.0	-33.0	6	0	-9	48.4	-49.1	7	7	-6	7.4	6.9
5	1	-3	21.4	-21.0	6	0	-10	40.6	40.2	7	7	-5	5.6	-6.8
5	1	-2	9.8	9.8	6	0	-11	5.6	6.2	7	7	-4	9.5	-9.4
6	10	2	9.6	-8.9	6	0	-12	33.5	33.4	7	5	-10	5.9	-6.0
6	10	0	15.2	14.5	6	0	-13	36.3	-35.4	7	5	-9	14.3	-15.0
6	8	5	14.0	14.8	6	0	-3	9.5	9.1	7	5	-7	12.7	12.5
6	8	4	6.6	6.4	6	2	-4	22.3	22.4	7	5	-5	17.7	-16.1
6	8	3	9.1	-8.5	6	2	-5	5.6	5.3	7	5	-4	17.4	-17.9
6	8	2	9.8	-10.1	6	2	-6	13.8	-14.3	7	5	-2	12.5	12.6
6	8	1	11.2	10.8	6	2	-8	20.3	20.5	7	3	-11	23.3	-23.3
6	8	0	22.0	20.0	6	2	-9	22.6	22.2	7	3	-9	13.0	12.8
6	6	6	30.9	33.0	6	2	-11	13.1	-12.8	7	3	-8	14.5	14.6
6	6	5	29.4	-30.1	6	2	13	14.5	13.6	7	3	-7	47.3	-50.5
6	6	3	20.0	19.8	6	4	-2	18.5	-17.7	7	3	-6	16.1	16.2
6	6	2	31.8	30.3	6	4	-3	6.0	-6.5	7	3	-5	10.5	-10.3
6	6	1	24.1	-23.5	6	4	-4	18.4	17.5	7	3	-4	43.7	43.0
6	6	-1	21.0	-21.5	6	4	-5	17.7	16.9	7	3	-3	42.7	-40.5
6	4	5	21.4	21.1	6	4	-8	7.3	7.4	7	3	-2	23.1	-24.2
6	4	4	8.8	9.0	6	4	-12	12.2	12.7	7	1	-11	6.2	8.2
6	4	3	13.1	-14.2	6	0	-2	75.0	74.2	7	1	-9	18.8	-18.2
6	4	2	12.7	-13.5	6	0	-3	21.9	-21.8	7	1	-7	10.5	11.1
6	4	1	15.3	15.3	6	0	-5	23.6	-23.7	7	1	-6	6.0	6.0
6	4	0	32.0	32.5	6	0	-6	31.4	30.7	7	1	-5	16.2	-15.9
6	4	-1	7.6	7.1	6	0	-7	20.5	20.1	7	1	-4	18.0	-17.9
6	2	9	14.6	15.4	6	0	-9	28.7	-30.3	7	1	-2	10.4	10.7
6	2	8	6.1	6.2	6	0	-10	32.3	33.5	8	4	0	6.9	8.2
6	2	7	10.7	-11.3	6	0	-12	13.8	-13.8	8	2	2	13.5	-13.7
6	2	6	8.3	-8.1	6	0	-14	14.1	13.5	8	2	0	17.2	15.9
6	2	5	18.0	18.0	6	0	-5	10.8	10.8	8	2	-1	19.8	18.1
6	2	4	17.5	18.4	6	0	-8	6.6	6.2	8	0	3	13.5	-12.7
6	2	2	8.9	-9.5	6	0	-9	9.7	8.5	8	0	2	45.5	44.7
6	2	1	6.7	6.1	6	0	-11	8.0	-7.1	8	0	1	11.3	-10.3
6	2	0	18.4	17.6	6	0	-12	10.2	10.3	8	0	0	9.9	8.3
6	0	9	43.9	-43.8	7	0	-1	6.5	-5.7	8	0	-1	41.3	-40.4
6	0	8	17.3	18.5	7	0	0	16.7	-16.7	8	0	-2	29.9	29.2
6	0	6	49.8	52.0	7	0	2	6.3	6.3	8	0	-3	20.8	20.3
6	0	5	31.3	-31.5	7	0	4	13.3	-13.5	8	0	-5	23.2	-23.2
6	0	4	11.2	-11.7	7	0	5	6.7	-6.6	8	0	-8	9.9	10.3
6	0	3	9.5	9.9	7	0	6	8.7	8.8	8	0	-8	28.6	28.7
6	0	2	35.8	34.4	7	0	8	30.2	32.4	8	2	-3	13.8	-13.7
6	0	1	18.8	-17.7	7	0	9	12.5	-14.4	8	2	-5	13.2	13.0
6	0	0	12.7	12.2	7	0	2	8.2	-10.1	8	2	-6	6.6	6.8
6	0	-1	23.2	-22.1	7	0	3	37.8	-38.1	8	4	-4	9.3	8.5
6	0	-2	86.1	80.7	7	0	4	44.9	45.1	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/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	12	-3	19.0	-18.6	3	3	-2	56.4	58.0	5	9	-1	32.9	-33.5
2	12	-3	24.1	-24.1	5	3	-2	22.7	-22.5	3	9	-1	68.2	-68.2
4	12	-3	26.6	-27.3	7	3	-2	15.4	-15.3	1	9	-1	49.9	-47.7
1	11	-3	21.2	-20.2	4	2	-2	20.0	-20.8	-1	9	-1	12.6	-12.3
2	10	-3	14.2	14.6	2	2	-2	40.4	41.7	-4	8	-1	15.9	16.6
3	9	-3	15.2	-14.3	0	2	-2	79.6	80.8	-2	8	-1	26.7	25.6
1	9	-3	27.2	-25.7	-3	1	-2	37.1	-37.9	0	8	-1	14.0	12.6
-1	9	-3	29.6	-28.3	1	1	-2	85.8	-85.6	2	8	-1	10.2	-10.2
-3	9	-3	45.9	-45.5	1	1	-2	63.4	-64.9	-3	7	-1	30.4	-30.3
-5	9	-3	37.2	-38.6	3	1	-2	19.0	-19.5	-5	7	-1	17.1	-17.6
2	8	-3	24.5	24.1	6	0	-2	72.0	71.9	-6	6	-1	21.0	-20.5
3	7	-3	25.3	-24.4	4	0	-2	98.8	100.0	-4	6	-1	33.1	-32.1
1	7	-3	42.4	-42.8	2	0	-2	24.5	-23.4	-2	6	-1	84.3	-83.1
-1	7	-3	24.1	-23.1	-2	0	-2	113.6	113.0	0	6	-1	56.2	-56.6
-3	7	-3	11.7	10.1	4	0	-2	27.3	27.7	2	6	-1	53.9	53.3
-6	6	-3	13.8	12.4	6	0	-2	33.5	32.4	4	6	-1	23.9	23.0
-2	6	-3	43.3	-42.8	8	0	-2	33.9	34.3	6	6	-1	19.1	-18.4
0	6	-3	33.4	-35.7	8	0	-2	11.1	12.7	3	5	-1	21.4	22.7
2	6	-3	65.7	-66.0	8	4	-2	13.9	-12.7	1	5	-1	15.0	16.6
4	6	-3	62.6	-64.2	2	4	-2	12.3	13.3	-1	5	-1	38.8	-39.0
3	5	-3	52.5	-53.1	0	4	-2	28.4	29.9	-3	5	-1	27.0	-27.9
1	5	-3	43.5	-44.8	-2	4	-2	50.8	52.1	-5	5	-1	16.7	-15.2
-1	5	-3	16.7	-16.9	-3	5	-2	30.4	-30.4	-6	4	-1	14.1	14.0
2	4	-3	46.4	47.0	-1	5	-2	58.4	-60.5	-4	4	-1	20.1	20.5
4	4	-3	23.5	23.6	1	5	-2	28.1	-28.8	-2	4	-1	53.0	53.5
7	3	-3	33.8	-34.8	3	5	-2	16.4	-16.4	0	4	-1	40.9	41.8
3	3	-3	20.4	-21.2	6	6	-2	59.5	60.2	2	4	-1	23.2	-24.1
1	3	-3	110.1	-111.9	4	6	-2	49.0	49.1	5	3	-1	51.3	-50.7
-1	3	-3	89.1	-87.6	0	6	-2	19.4	19.7	3	3	-1	155.0	-155.4
-3	3	-3	72.8	-70.8	-2	6	-2	25.3	24.6	1	3	-1	124.2	-123.7
-5	3	-3	76.7	-75.9	-4	6	-2	32.2	30.0	-1	3	-1	25.0	23.5
-7	3	-3	32.0	-32.6	-6	6	-2	26.7	26.4	-3	3	-1	20.3	-20.9
-4	2	-3	22.2	-21.8	-3	7	-2	14.7	-15.0	-5	3	-1	29.4	-28.5
-2	2	-3	24.5	-25.7	-1	7	-2	33.0	-33.9	-7	3	-1	15.0	-14.7
0	2	-3	59.3	60.4	1	7	-2	44.1	-45.7	-4	2	-1	52.4	51.8
2	2	-3	15.7	17.3	2	8	-2	13.0	11.0	-2	2	-1	36.1	37.1
4	2	-3	15.2	16.9	0	8	-2	24.6	23.7	0	2	-1	11.1	12.0
5	1	-3	20.1	-19.7	-2	8	-2	23.2	23.4	2	2	-1	41.5	42.3
3	1	-3	61.0	-63.4	-3	9	-2	18.4	15.9	4	2	-1	13.3	-14.2
1	1	-3	75.9	-78.7	-1	9	-2	31.9	31.0	3	1	-1	21.4	23.2
-1	1	-3	40.3	-40.2	3	9	-2	64.7	62.8	1	1	-1	13.7	12.4
-7	0	-3	83.2	-84.4	0	9	-2	18.0	19.0	-1	1	-1	40.3	-39.7
-2	0	-3	110.7	-115.0	0	10	-2	20.0	20.0	-3	1	-1	40.8	-41.7
2	0	-3	46.9	-49.1	-1	11	-2	17.5	-18.1	-5	1	-1	21.7	-22.1
4	0	-3	83.6	-84.6	1	11	-2	22.7	-20.7	-6	0	-1	19.6	-18.4
6	0	-3	38.5	-38.1	-1	13	-2	15.4	-14.2	-4	0	-1	68.0	-68.3
5	3	-3	14.0	-13.8	-4	12	-1	16.2	-16.6	-2	0	-1	101.3	-101.8
-3	3	-2	34.8	36.6	-2	12	-1	32.7	-31.3	0	0	-1	64.7	-64.3
-1	3	-2	47.9	48.8	-4	10	-1	16.9	15.2	2	0	-1	40.4	39.5
1	3	-2	98.4	100.6	-2	10	-1	16.6	16.5	4	0	-1	55.1	54.1

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
6	0	-1	20.8	-20.9	7	3	4	32.1	33.0	5	5	5	19.0	-19.0
8	0	-1	29.5	-30.2	-2	2	4	21.4	-21.4	-3	5	5	15.4	14.5
7	3	0	26.4	26.6	-4	2	4	33.5	35.1	-6	4	5	13.9	14.0
5	3	0	67.1	65.7	-6	2	4	19.8	19.6	0	4	5	16.9	17.5
3	3	0	57.3	57.6	-5	1	4	29.6	-29.8	4	4	5	31.4	31.1
1	3	0	40.1	-39.6	-3	1	4	34.1	-35.3	5	3	5	17.7	16.2
6	2	0	15.1	15.3	-1	1	4	20.8	-19.4	-1	3	5	106.8	-106.7
4	2	0	33.9	34.2	4	0	4	88.6	88.0	-1	3	5	127.2	-129.1
2	2	0	43.7	43.4	2	0	4	131.8	129.9	-3	3	5	69.6	-71.1
0	2	0	32.4	-33.1	0	0	4	66.2	63.4	-5	3	5	31.5	-30.3
8	2	0	12.4	11.9	-2	0	4	87.2	87.7	-4	2	5	15.6	15.7
5	1	0	19.0	-18.9	-4	0	4	26.7	26.0	-2	2	5	11.9	-12.3
1	1	0	28.6	28.8	-7	1	4	16.7	-14.7	4	2	5	46.5	47.3
7	1	0	13.6	-13.3	2	4	4	20.1	-19.6	5	2	5	24.8	24.0
6	0	0	16.7	16.4	0	4	4	21.5	-22.8	5	1	5	18.8	-19.4
4	0	0	12.4	10.4	-2	4	4	26.6	26.0	3	1	5	17.2	-17.4
2	0	0	125.0	125.4	-4	4	4	14.5	14.1	-3	1	5	12.2	12.3
6	4	0	26.1	26.0	-6	4	4	15.7	15.1	-8	0	5	17.2	-18.0
4	4	0	19.0	19.1	-5	5	4	19.0	-19.2	-6	0	5	17.2	-17.2
0	4	0	42.0	42.7	-3	5	4	28.0	-28.2	-4	0	5	42.4	-43.5
5	5	0	17.0	-17.4	-1	5	4	16.3	-15.1	-2	0	5	29.0	29.3
3	5	0	11.0	10.5	1	5	4	18.1	19.3	0	0	5	92.8	90.9
1	5	0	14.6	14.6	4	6	4	43.8	44.7	2	0	5	54.2	-54.5
4	6	0	12.0	13.3	2	6	4	100.4	99.0	4	0	5	67.4	-66.1
2	6	0	98.3	98.1	0	6	4	69.8	69.9	6	0	5	26.5	-27.4
0	6	0	153.4	152.8	-2	6	4	28.3	26.4	-7	1	5	12.2	-13.0
1	7	0	23.9	25.1	-4	6	4	28.3	27.7	6	2	5	14.2	14.3
4	8	0	15.4	13.8	-5	7	4	25.8	-25.2	-3	3	0	29.3	-29.9
6	8	0	16.5	15.3	-3	7	4	13.8	-14.7	-1	3	6	51.9	53.9
5	9	0	31.9	32.5	2	8	4	11.8	-9.8	1	3	6	124.8	124.0
3	9	0	37.1	35.4	0	8	4	13.9	-11.3	3	3	6	57.4	56.0
1	9	0	23.2	-23.2	-4	8	4	13.7	11.0	4	2	6	25.4	26.2
1	11	0	12.7	13.0	-5	9	4	25.9	25.1	2	2	6	55.1	55.2
2	12	0	30.3	31.8	-3	9	4	18.2	17.2	0	2	6	20.7	21.2
0	12	0	56.9	56.1	-1	9	4	13.0	11.3	-2	2	6	32.3	33.0
-3	7	1	10.1	10.3	3	9	4	17.5	-18.2	-3	1	6	15.0	14.4
-5	7	1	12.3	10.8	4	12	4	20.8	21.0	1	1	6	32.1	-32.2
5	3	2	15.1	12.7	2	12	4	35.0	37.3	3	1	6	21.9	-22.1
2	10	2	12.8	13.0	0	12	4	25.3	24.6	6	0	6	41.1	42.1
-3	13	3	15.4	-14.4	1	9	5	43.5	-43.0	4	0	6	30.9	30.3
-5	7	3	15.9	-15.9	-1	9	5	73.9	-72.7	2	0	6	14.6	-15.4
-5	5	3	12.7	-12.4	-3	9	5	32.4	-30.8	0	0	6	49.8	48.1
0	4	3	10.2	-11.3	-5	9	5	13.5	-13.3	-2	0	6	105.2	107.3
-7	3	4	35.7	33.8	-1	7	5	22.6	21.9	-4	0	6	101.4	101.4
-5	3	4	32.5	32.3	-6	6	5	21.2	-20.3	-6	0	6	49.1	48.1
-3	3	4	34.4	36.6	-4	6	5	11.3	-11.9	-7	3	6	15.5	14.6
-1	3	4	52.1	54.0	0	6	5	30.4	29.6	4	4	6	16.4	15.6
1	3	4	29.4	-28.4	2	6	5	15.4	-15.3	2	4	6	35.9	34.7
3	3	4	29.9	-29.2	4	6	5	57.1	-56.3	0	4	6	55.4	50.2
5	3	4	24.6	23.0	6	6	5	22.7	-23.9	-3	5	6	17.8	18.1

Table 8. Observed (FO) and calculated (FC) structure factors for sample 4. Tag 15-3.

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-1	1	-1	37.9	-38.1	2	0	42.3	41.3	-1	5	2	27.0	-26.9	
1	1	-1	12.3	12.2	2	0	30.7	30.5	0	4	2	25.6	20.0	
3	1	-1	21.6	22.3	2	0	14.1	12.3	2	4	2	47.5	47.2	
0	0	-1	21.6	-22.2	1	0	16.3	-16.7	3	3	2	31.6	30.8	
6	0	-1	17.8	-17.3	1	0	27.3	27.9	1	3	2	45.1	46.5	
4	0	-1	52.9	51.0	0	0	120.1	120.7	-1	3	2	95.2	96.9	
2	0	-1	39.4	38.7	0	0	8.7	7.5	0	2	2	74.4	77.3	
0	0	-1	57.6	-50.7	0	0	13.7	13.4	4	2	2	9.5	9.9	
4	2	-1	13.3	-12.5	1	1	37.3	-39.1	3	1	2	34.1	-34.3	
2	2	-1	41.2	40.5	1	1	17.3	-19.0	1	1	2	80.4	-81.5	
0	2	-1	11.8	12.1	0	1	14.6	-13.4	-1	1	2	60.1	-62.2	
-1	3	-1	25.4	24.5	0	1	61.6	-60.1	2	0	2	104.6	103.6	
1	3	-1	118.5	-119.6	0	1	99.1	-98.0	4	0	2	24.6	23.7	
3	3	-1	150.1	-148.4	2	1	44.4	46.0	6	0	2	23.8	24.3	
5	3	-1	44.0	-44.2	2	1	34.6	35.0	8	0	2	22.9	22.0	
2	4	-1	23.0	-23.0	3	1	10.9	-16.6	-1	1	3	73.3	-75.2	
0	4	-1	39.2	40.2	3	1	24.1	-25.0	1	1	3	37.6	-37.1	
-1	5	-1	36.6	-37.8	4	1	18.8	18.3	4	0	3	9.6	8.1	
1	5	-1	15.9	17.0	4	1	50.4	50.2	2	0	3	48.0	-49.3	
3	5	-1	21.7	22.1	5	1	24.4	-25.0	0	0	3	110.7	-110.7	
6	6	-1	14.1	-14.6	5	1	13.4	-12.5	4	2	3	18.5	-18.7	
4	6	-1	21.6	19.7	6	1	13.9	-15.3	2	2	3	24.7	-24.8	
2	6	-1	51.8	50.8	6	1	27.2	-27.2	0	2	3	55.4	56.6	
0	6	-1	53.5	-53.0	6	1	70.6	-76.8	-1	3	3	186.4	-186.8	
5	7	-1	10.9	9.5	7	1	27.2	-26.7	1	3	3	83.3	-82.2	
0	8	-1	12.4	12.2	7	1	15.7	-14.3	3	3	3	62.0	-60.6	
-1	9	-1	11.2	-11.8	8	1	14.4	13.2	5	3	3	56.9	-59.1	
1	9	-1	44.0	-42.5	8	1	23.5	22.4	7	3	3	22.4	-22.4	
3	9	-1	56.5	-58.7	10	1	13.3	12.4	0	4	3	10.7	-11.7	
5	9	-1	27.8	-27.9	11	1	12.4	-12.7	-1	5	3	41.0	-41.8	
0	12	0	45.0	47.3	12	1	14.1	-12.7	1	5	3	15.7	-15.7	
1	11	0	13.0	12.0	12	1	27.1	-26.0	2	6	3	38.8	-38.5	
5	9	0	26.8	25.8	13	2	12.6	-11.7	0	6	3	31.4	-32.7	
3	9	0	32.0	31.6	11	2	19.6	-18.6	-1	7	3	39.0	-40.0	
1	9	0	18.1	-19.8	9	2	17.3	16.7	1	7	3	22.0	-20.9	
1	7	0	23.4	24.4	9	2	11.7	10.7	-1	9	3	25.0	-23.8	
0	6	0	147.7	146.3	9	2	12.0	12.4	1	9	3	27.1	-25.6	
2	6	0	93.5	91.8	9	2	28.2	27.1	3	9	3	37.8	-37.2	
4	6	0	11.5	11.1	9	2	57.6	57.0	5	9	3	26.9	-27.9	
5	5	0	15.3	-14.5	8	2	22.0	21.0	-1	11	3	17.0	-17.1	
3	5	0	11.5	9.9	8	2	20.1	19.6	2	12	3	11.7	-10.8	
1	5	0	13.8	15.0	7	2	12.2	-12.4	0	12	3	14.3	-16.1	
0	4	0	40.4	40.3	7	2	31.0	-31.0	-1	13	3	8.4	-8.4	
4	4	0	16.0	16.9	7	2	42.0	-43.3	0	12	4	20.2	20.4	
6	4	0	19.2	21.2	6	2	17.4	16.9	2	12	4	27.6	28.0	
7	3	0	18.9	19.8	6	2	22.3	21.8	4	12	4	15.0	15.0	
5	3	0	57.0	56.3	6	2	25.7	25.6	3	9	4	13.4	-13.0	
3	3	0	54.5	52.6	6	2	18.5	18.9	0	8	4	11.1	-10.1	
1	3	0	39.7	-38.3	5	2	27.6	-27.4	0	6	4	64.3	63.1	
0	2	0	32.4	-32.6	5	2	54.7	-56.2	2	6	4	86.4	85.2	

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
4	6	4	34.3	35.7	5	6	25.8	-25.7	3	1	9	12.4	-10.7	
1	5	4	17.3	18.4	5	6	8.8	-9.7	6	0	9	18.5	-17.5	
-1	5	4	13.7	-14.5	4	6	50.0	50.0	0	0	9	25.2	-25.4	
0	4	4	20.7	-22.3	4	6	30.2	29.6	-1	3	9	63.0	-61.1	
2	4	4	17.9	-17.3	3	6	45.4	46.0	1	3	9	51.2	-50.2	
7	3	4	20.6	22.2	3	6	114.7	113.2	3	3	9	27.3	-28.0	
5	3	4	17.2	17.9	3	6	48.5	49.9	0	4	9	20.4	-20.1	
3	3	4	26.6	-26.6	2	6	19.5	20.3	-1	9	9	25.2	-27.7	
-1	3	4	27.4	-26.7	2	6	48.2	47.2	1	9	9	19.2	-21.0	
-1	1	4	48.6	50.0	2	6	18.8	19.2	3	9	9	16.1	-18.0	
0	0	4	18.3	-18.4	1	6	18.4	-17.2	1	9	10	11.6	10.0	
2	0	4	58.8	58.4	1	6	28.6	-28.0	1	7	10	13.7	-12.3	
4	0	4	116.6	117.3	0	8	42.2	41.6	0	6	10	29.5	30.3	
3	1	5	70.7	70.1	0	6	15.0	-16.7	3	3	10	17.6	16.5	
5	1	5	14.8	-13.8	0	6	23.1	24.2	3	3	10	29.7	29.4	
6	0	5	13.9	-13.7	0	6	27.3	27.9	1	3	10	10.4	9.5	
4	0	5	17.3	-18.6	1	7	33.6	-34.6	0	2	10	11.2	11.4	
2	0	5	53.6	-53.8	1	7	24.6	-24.2	2	2	10	16.9	15.9	
0	0	5	45.2	-45.6	0	7	57.1	-56.9	3	1	10	11.3	-11.6	
0	0	5	88.1	87.0	2	7	31.2	32.1	1	1	10	14.1	-13.3	
-1	1	5	9.0	9.5	3	7	14.5	15.8	0	0	10	40.7	39.3	
4	2	5	19.3	19.3	3	7	33.6	-33.1	-1	1	11	15.8	-15.4	
2	2	5	39.7	40.9	3	7	49.6	-49.6	1	1	11	11.4	-11.6	
-1	3	5	122.0	-122.8	0	3	22.3	-23.2	2	0	11	34.4	-32.9	
1	3	5	99.3	-96.9	2	4	13.2	13.8	0	0	11	37.9	-36.4	
5	3	5	12.6	13.2	4	7	38.0	38.4	2	2	11	17.5	17.3	
4	4	5	24.6	24.1	5	7	22.7	-22.1	0	2	11	14.4	14.4	
0	4	5	15.9	15.8	0	5	21.7	-22.7	1	3	11	11.6	11.5	
5	5	5	12.1	-12.9	0	6	50.0	-48.0	5	3	11	16.1	-15.4	
6	6	5	16.3	-15.3	7	7	25.0	-25.6	0	4	11	10.5	20.5	
4	6	5	43.4	-43.5	8	7	10.7	20.1	-1	5	11	13.7	-15.0	
2	6	5	12.6	-12.5	8	7	14.9	13.3	-2	6	11	16.0	-18.2	
0	6	5	28.2	27.3	1	9	19.5	-21.2	0	6	11	31.3	-32.1	
-1	7	5	19.5	20.6	3	9	20.4	-22.8	0	8	11	12.9	11.4	
3	7	5	11.9	-11.9	11	7	13.8	-12.8	-1	9	12	19.1	19.4	
-1	9	5	64.7	-64.2	12	7	16.1	-17.2	0	6	12	11.3	10.1	
1	9	5	37.4	-36.1	12	8	17.4	18.2	2	6	12	25.0	27.9	
0	10	6	13.3	12.1	7	8	15.7	-16.0	0	4	12	14.1	14.3	
2	10	6	17.2	15.1	0	6	52.2	52.7	-1	3	12	37.0	36.8	
3	9	6	30.3	28.9	6	8	26.9	26.6	-1	1	12	11.5	-10.2	
-1	9	6	45.0	45.5	6	8	18.4	18.4	0	0	12	26.3	24.4	
-1	9	6	18.6	19.0	6	8	10.8	-10.5	2	0	12	36.1	35.7	
0	8	6	23.1	23.4	2	8	23.0	-22.0	4	0	12	18.3	17.6	
2	8	6	18.0	18.4	0	8	15.0	-15.7	0	0	13	10.0	17.5	
3	7	6	16.5	-18.1	3	8	65.8	65.1	-1	3	13	39.7	-39.0	
1	7	6	12.2	-10.9	0	8	49.7	53.9	1	3	13	24.1	-25.4	
4	6	6	19.5	19.9	1	8	21.8	21.5	-1	9	13	16.9	-18.0	
6	6	6	16.3	16.8	0	8	12.8	11.1						

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-2	12	-3	13.2	-13.3	-2	8	-3	57.0	-1.0	-5	9	-2	14.6	14.5
0	12	-3	19.8	-19.1	0	0	-3	121.5	-1.6	-3	9	-2	17.1	17.4
2	12	-3	23.8	-23.5	2	0	-3	52.7	-1.5	-1	9	-2	32.4	32.1
4	12	-3	25.8	-26.3	4	0	-3	89.5	-1.5	1	9	-2	63.3	62.0
3	11	-3	12.4	-11.5	6	0	-3	48.5	-1.1	3	9	-2	20.9	21.1
1	11	-3	19.1	-18.2	-5	3	-2	14.4	0.9	0	10	-2	18.3	18.4
-1	11	-3	8.6	-9.3	-3	3	-2	38.6	0.3	-1	11	-2	14.1	-14.0
2	10	-3	12.2	12.4	-1	3	-2	53.1	0.0	1	11	-2	19.0	-18.8
3	9	-3	15.9	-14.8	1	3	-2	105.7	0.2	4	12	-2	19.5	21.3
1	9	-3	27.3	-26.2	3	3	-2	61.5	0.6	-2	12	-2	11.1	10.6
-1	9	-3	30.4	-28.6	5	3	-2	20.7	0.5	-1	13	-2	12.9	-12.1
-3	9	-3	43.5	-43.5	7	3	-2	13.3	0.3	-4	12	-1	16.6	-16.5
-5	9	-3	35.3	-36.8	4	2	-2	26.8	0.3	-2	12	-1	30.4	-30.0
-4	8	-3	10.8	-9.8	2	2	-2	41.2	0.0	0	12	-1	16.8	-17.1
2	8	-3	22.4	22.4	0	2	-2	77.7	0.2	-3	11	-1	14.4	-14.7
4	8	-3	11.5	-11.9	-4	2	-2	12.0	0.1	-4	10	-1	13.9	13.8
5	7	-3	14.2	-14.5	-3	1	-2	37.2	0.0	-2	10	-1	14.4	14.9
3	7	-3	22.9	-23.0	-1	1	-2	83.7	0.0	5	9	-1	32.4	-32.4
1	7	-3	40.3	-40.6	1	1	-2	63.2	0.4	3	9	-1	67.8	-66.6
-1	7	-3	22.2	-21.5	3	1	-2	17.8	0.3	1	9	-1	48.1	-47.6
-2	6	-3	44.3	-44.5	5	1	-2	8.6	0.3	-1	9	-1	13.5	-13.4
0	6	-3	36.4	-38.1	8	0	-2	26.3	0.5	-4	8	-1	14.3	14.8
2	6	-3	68.7	-69.1	6	0	-2	74.0	0.9	-2	8	-1	23.8	23.9
4	6	-3	67.5	-65.9	4	0	-2	103.9	0.7	0	8	-1	12.5	11.8
6	6	-3	19.8	-20.0	2	0	-2	19.7	0.7	2	8	-1	11.4	-11.6
5	5	-3	12.7	-12.3	-2	0	-2	114.0	0.4	3	7	-1	11.4	11.1
3	5	-3	51.4	-52.2	-4	0	-2	29.0	0.1	-3	7	-1	28.7	-29.0
-1	5	-3	43.1	-44.2	-6	0	-2	32.9	0.1	-5	7	-1	16.2	-16.2
-4	4	-3	17.1	-17.4	-8	0	-2	34.7	0.2	-6	6	-1	22.0	-22.0
0	4	-3	11.3	-11.4	8	4	-2	13.1	0.1	-4	6	-1	35.0	-34.1
2	4	-3	11.9	-12.7	2	4	-2	12.2	0.1	-2	6	-1	84.9	-85.2
4	4	-3	45.2	46.3	0	4	-2	27.1	0.8	0	6	-1	58.1	-59.2
2	4	-3	22.8	22.5	-2	4	-2	50.0	0.9	2	6	-1	50.6	50.2
7	3	-3	35.8	-35.7	-3	5	-2	28.6	0.3	4	6	-1	20.6	20.1
5	3	-3	15.5	-14.8	-1	5	-2	56.9	0.7	6	6	-1	19.2	-19.9
3	3	-3	22.9	-22.6	1	5	-2	27.2	0.6	3	5	-1	22.4	23.3
1	3	-3	113.7	-113.8	3	5	-2	14.8	0.8	1	5	-1	15.8	16.7
-1	3	-3	88.1	-89.0	6	8	-2	11.0	0.8	-1	5	-1	37.2	-38.2
-3	3	-3	71.7	-72.1	4	6	-2	51.5	0.4	-3	5	-1	28.0	-27.7
-5	3	-3	75.5	-75.6	2	6	-2	11.8	0.7	-5	5	-1	16.2	-15.7
-7	3	-3	32.4	-32.1	0	6	-2	21.1	0.6	-6	4	-1	13.4	13.3
-4	2	-3	21.5	-21.9	-2	6	-2	26.0	0.2	-4	4	-1	19.6	19.4
-2	2	-3	25.7	-26.8	-4	6	-2	31.3	0.3	-2	4	-1	50.7	51.8
0	2	-3	57.5	59.0	-6	6	-2	25.6	0.9	0	4	-1	39.3	41.4
2	2	-3	15.0	15.7	-3	7	-2	14.4	0.4	2	4	-1	23.5	-25.4
4	2	-3	16.5	16.9	-1	7	-2	31.6	0.1	5	3	-1	51.6	-51.8
5	1	-3	19.4	-18.8	1	7	-2	42.5	0.1	3	3	-1	156.6	-157.3
3	1	-3	63.5	-63.4	2	8	-2	11.6	0.3	1	3	-1	125.6	-125.9
1	1	-3	77.4	-77.4	0	8	-2	23.1	0.6	-1	3	-1	19.6	18.3
-1	1	-3	39.1	-40.3	-2	8	-2	22.3	0.7	-3	3	-1	22.7	-22.8

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-5	3	-1	29.5	-29.2	3	9	0	36.3	0.8	0	6	4	69.9	70.3
-7	3	-1	14.5	-15.2	1	9	0	19.2	0.1	-2	6	4	27.0	27.2
-4	2	-1	50.6	50.7	1	11	0	13.4	0.2	-4	6	4	28.0	27.9
-2	2	-1	35.7	35.9	2	12	0	30.2	0.0	-5	7	4	25.0	-23.9
0	2	-1	9.8	11.2	0	12	0	51.9	0.8	-3	7	4	14.1	-14.0
2	2	-1	41.5	41.9	-2	12	1	11.5	0.8	2	8	4	9.8	-10.0
4	2	-1	14.4	-15.3	8	0	1	12.5	0.1	0	8	4	11.3	-10.9
8	2	-1	12.2	12.3	6	4	2	9.8	0.1	-6	8	4	10.7	10.2
3	1	-1	23.2	24.6	-5	7	2	10.0	0.1	-5	9	4	25.6	25.4
1	1	-1	13.0	12.8	-5	9	2	14.3	0.1	-3	9	4	18.9	18.5
-1	1	-1	39.1	-39.1	-1	13	3	9.1	0.1	-1	9	4	13.7	13.5
-3	1	-1	40.5	-41.9	-3	13	3	14.1	0.4	3	9	4	13.8	-15.1
-5	1	-1	21.9	-22.3	3	7	3	9.4	0.8	-5	11	4	13.7	-11.8
-6	0	-1	20.1	-20.5	6	6	3	11.5	0.9	4	12	4	19.8	19.9
-4	0	-1	72.6	-72.0	-7	3	4	34.5	0.7	2	12	4	33.5	34.2
-2	0	-1	107.1	-106.8	-5	3	4	11.5	0.9	0	12	4	23.8	23.0
0	0	-1	65.7	-67.5	-3	3	4	35.0	0.3	-2	12	4	14.2	12.8
2	0	-1	30.2	34.0	-1	3	4	39.3	0.8	-1	11	5	12.1	11.0
4	0	-1	52.5	52.4	1	3	4	50.1	0.8	1	9	5	42.1	-41.8
6	0	-1	24.1	-23.7	5	3	4	23.2	0.4	-1	9	5	71.0	-69.3
8	0	-1	33.0	-31.4	3	3	4	27.3	0.0	-3	9	5	29.8	-30.2
7	3	0	28.1	27.6	5	3	4	26.1	0.9	-5	9	5	14.6	-13.9
5	3	0	67.7	68.0	7	3	4	33.5	0.0	-5	9	5	16.6	17.2
3	3	0	61.4	61.8	6	2	4	15.0	0.6	4	8	5	14.9	-14.2
1	3	0	35.3	-33.5	4	2	4	10.1	0.1	3	7	5	20.1	20.6
8	2	0	12.2	11.8	-2	2	4	20.8	0.5	-1	7	5	21.7	-22.2
6	2	0	14.4	14.7	-4	2	4	33.2	0.6	-6	6	5	14.9	-14.5
4	2	0	32.5	32.8	-8	2	4	13.6	0.3	0	6	5	25.2	25.6
2	2	0	44.0	44.3	-7	1	4	28.8	0.0	2	6	5	17.0	-16.4
0	2	0	33.7	-32.8	-5	1	4	33.7	0.5	-4	6	5	54.4	-55.3
5	1	0	18.6	-18.1	-3	1	4	19.1	0.1	6	6	5	22.8	-23.5
1	1	0	29.1	29.4	5	1	4	9.2	0.1	5	5	5	16.6	-17.2
7	1	0	13.7	-13.1	4	0	4	87.5	0.0	3	5	5	11.5	-10.1
6	0	0	17.0	16.7	2	0	4	134.7	0.8	-3	5	5	13.9	14.1
4	0	0	13.3	12.3	0	0	4	66.8	0.3	-7	5	5	12.3	-12.3
2	0	0	128.6	127.7	-2	0	4	88.2	0.3	-6	4	5	14.3	13.3
6	4	0	25.0	24.9	-4	0	4	26.5	0.5	0	4	5	15.2	15.6
4	4	0	18.6	18.8	4	4	4	11.8	0.2	4	4	5	30.3	29.6
0	4	0	42.1	43.1	2	4	4	19.5	0.1	4	4	5	14.6	15.2
5	5	0	16.7	-18.4	0	4	4	21.6	0.6	7	3	5	12.1	-12.4
3	5	0	10.3	10.8	-2	4	4	25.5	0.4	5	3	5	15.6	15.1
1	5	0	16.0	16.9	-4	4	4	13.5	0.0	1	3	5	106.6	-107.2
4	6	0	15.0	14.1	-6	4	4	14.5	0.6	-1	3	5	128.6	-130.0
2	6	0	99.0	99.0	-7	5	4	11.7	0.7	-3	3	5	71.5	-72.4
0	6	0	151.4	152.4	-5	5	4	17.8	0.7	-5	3	5	32.0	-31.5
3	7	0	9.3	-8.0	-3	5	4	27.2	0.3	-7	3	5	11.9	-13.0
1	7	0	23.9	24.8	-1	5	4	13.4	0.3	-4	2	5	13.7	13.9
4	8	0	13.2	12.8	1	5	4	19.3	0.7	-2	2	5	12.7	-14.0
6	8	0	14.8	14.3	4	6	4	44.1	1.4	0	2	5	9.4	-9.7
5	9	0	32.7	32.5	2	6	4	99.5	0.7	2	2	5	45.2	45.1

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	13	0	7.5	8.0	-4	12	1	14.1	14.5	-2	2	1	40.2	41.2
2	12	0	31.4	32.6	-5	11	1	7.7	8.4	-4	2	1	14.4	-15.7
0	12	0	61.4	59.0	-3	11	1	9.3	8.9	-8	2	1	13.6	14.2
1	11	0	15.4	14.9	3	11	1	16.8	-16.1	-5	1	1	6.0	6.5
6	10	0	10.4	11.1	5	11	1	8.6	-9.0	-3	1	1	23.2	24.7
4	10	0	9.5	10.1	4	10	1	15.5	15.6	-1	1	1	13.1	14.3
0	10	0	5.9	-6.5	2	10	1	17.6	17.1	1	1	1	37.7	-38.2
5	9	0	34.3	34.7	-5	9	1	33.0	-33.7	3	1	1	30.8	-40.7
3	9	0	35.8	36.6	-3	9	1	63.3	-69.0	5	1	1	20.7	-21.0
1	9	0	26.7	-27.4	1	9	1	45.9	-45.0	6	0	1	15.9	-16.2
6	8	0	15.9	16.0	9	1	1	0.1	-7.7	4	0	1	62.4	-64.1
4	8	0	13.7	13.5	9	1	1	5.1	5.0	2	0	1	92.0	-93.4
7	7	0	6.6	-7.4	9	1	1	0.7	-9.0	0	0	1	54.9	-52.1
5	7	0	7.9	-8.3	8	1	1	0.4	8.3	-2	0	1	47.3	47.1
3	7	0	8.4	-8.1	1	8	1	17.8	17.9	-4	0	1	58.9	60.0
1	7	0	26.7	26.4	7	8	1	27.1	27.1	-6	0	1	17.7	-19.6
4	6	0	7.3	8.0	7	8	1	13.2	13.2	-8	0	1	30.6	-32.3
2	6	0	92.6	93.4	2	8	1	10.5	-10.9	0	14	2	7.6	7.6
0	6	0	147.0	140.9	7	7	1	5.3	-5.6	3	13	2	7.1	-7.1
7	5	0	13.0	-12.9	7	7	1	12.2	12.2	1	13	2	15.1	-14.7
5	5	0	17.9	-18.0	1	7	1	10.8	11.3	2	12	2	8.4	8.7
3	5	0	11.1	11.9	3	7	1	30.4	-30.8	4	12	2	7.8	8.4
1	5	0	14.3	15.3	1	7	1	17.7	-17.7	3	11	2	7.2	-7.1
0	4	0	6.5	7.0	6	1	1	19.7	-19.3	1	11	2	17.5	-17.1
8	4	0	28.2	27.5	6	1	1	30.0	-30.1	-1	11	2	23.9	-23.1
4	4	0	18.9	19.2	6	1	1	80.4	-81.1	-2	10	2	9.3	9.1
0	4	0	41.0	41.6	6	1	1	51.5	-52.7	0	10	2	20.3	20.2
7	3	0	27.5	27.1	6	1	1	59.1	59.3	2	10	2	12.5	12.7
5	3	0	66.4	66.1	6	1	1	27.1	27.7	5	9	2	13.2	13.4
3	3	0	52.1	53.3	5	1	1	25.1	25.7	3	9	2	13.7	13.7
1	3	0	47.6	-47.5	5	1	1	18.5	19.4	1	9	2	29.3	29.2
8	2	0	12.3	12.4	5	1	1	36.4	-38.0	-1	9	2	64.7	63.5
6	2	0	15.2	15.6	5	1	1	26.4	-26.8	-3	9	2	18.2	18.8
4	2	0	32.8	34.2	5	1	1	14.0	-14.0	-5	9	2	18.4	-18.8
2	2	0	39.8	40.8	4	1	1	13.9	13.4	-6	8	2	10.2	-10.3
0	2	0	35.5	-37.0	4	1	1	20.1	20.2	-2	8	2	9.7	9.9
7	1	0	13.8	-13.8	4	1	1	52.5	53.7	0	8	2	22.8	22.7
5	1	0	18.3	-18.9	4	1	1	39.3	40.2	2	8	2	21.9	21.9
3	1	0	5.2	5.6	4	1	1	25.7	-26.4	6	8	2	6.8	-7.1
1	1	0	30.1	30.0	3	1	1	47.5	-47.1	3	7	2	13.3	-12.8
6	0	0	12.7	12.1	3	1	1	149.8	-150.6	1	7	2	31.2	-32.3
2	0	0	113.2	115.4	3	1	1	115.1	-114.3	-1	7	2	45.4	-45.9
2	14	1	9.5	9.5	3	1	1	30.3	35.0	-0	7	2	10.7	10.5
-3	13	1	9.8	9.7	3	1	1	11.7	-12.0	-8	6	2	61.0	61.4
1	13	1	8.6	-9.2	3	1	1	25.0	-24.6	-4	6	2	45.5	45.6
3	13	1	7.0	-8.2	3	1	1	12.2	-12.6	0	6	2	11.5	11.9
4	12	1	16.9	-16.9	2	1	1	6.1	6.2	2	6	2	19.9	19.6
2	12	1	34.4	-33.7	2	1	1	51.2	52.8	4	6	2	27.0	26.8
0	12	1	18.5	-17.7	2	1	1	34.4	36.7	6	6	2	24.9	25.4
-2	12	1	19.3	18.0	2	1	1	11.2	10.3	5	5	2	4.8	4.8

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
3	5	2	30.0	-30.2	11	3	3	7.4	-8.7	5	3	3	74.9	-72.9
1	5	2	58.9	-60.4	11	3	3	11.9	-12.0	7	3	3	30.9	-31.3
-1	5	2	27.3	-28.6	11	3	3	20.5	-19.7	4	2	3	22.7	-23.2
-3	5	2	16.6	-17.1	11	3	3	9.5	-9.1	2	2	3	24.8	-26.3
-5	5	2	4.9	5.3	11	3	3	7.7	7.9	0	2	3	58.7	57.9
-7	5	2	9.4	9.5	10	3	3	9.2	-9.2	-2	2	3	14.9	16.1
-6	4	2	14.8	-14.6	10	3	3	9.1	-8.3	-4	2	3	15.3	15.8
-4	4	2	7.0	6.9	10	3	3	6.8	6.7	-6	2	3	8.4	7.7
-2	4	2	11.3	12.0	10	3	3	13.4	13.4	-8	2	3	10.6	-10.0
0	4	2	27.0	28.7	10	3	3	8.4	9.1	-5	1	3	19.1	-19.0
2	4	2	49.8	50.6	9	3	3	11.7	-11.5	-3	1	3	60.0	-61.8
4	4	2	4.7	-4.5	9	3	3	24.0	-23.2	-1	1	3	74.9	-75.1
6	4	2	10.9	-10.8	9	3	3	26.5	-25.5	1	1	3	37.7	-36.5
5	3	2	8.9	9.4	9	3	3	45.2	-44.4	3	1	3	5.4	-5.3
3	3	2	29.0	31.0	9	3	3	38.2	-39.0	5	1	3	4.7	4.9
1	3	2	40.6	41.8	8	3	3	6.7	-6.3	8	0	3	9.0	-10.1
-1	3	2	92.2	92.4	8	3	3	10.7	-10.6	6	0	3	7.0	7.5
-3	3	2	52.2	53.1	8	3	3	4.4	4.1	4	0	3	14.6	15.2
-5	3	2	27.7	-27.5	8	3	3	23.9	24.0	2	0	3	43.7	-45.7
-6	2	2	5.5	-5.8	8	3	3	12.9	13.2	0	0	3	107.7	-104.7
-4	2	2	22.1	-23.3	7	3	3	16.1	-16.3	-2	0	3	40.9	-41.2
-2	2	2	38.3	39.4	7	3	3	24.0	-23.8	-4	0	3	80.7	-80.9
0	2	2	78.1	79.5	7	3	3	41.6	-42.1	-6	0	3	38.0	-37.5
4	2	2	10.0	9.8	7	3	3	22.8	-23.1	0	14	4	5.9	-5.6
8	2	2	7.1	-7.0	7	3	3	10.5	10.6	1	13	4	9.4	8.9
0	2	2	9.8	-9.9	6	3	3	14.9	14.6	-3	13	4	5.8	-6.1
3	1	2	34.6	-35.7	6	3	3	4.8	4.9	-2	12	4	10.8	11.1
-1	1	2	01.9	-03.0	6	3	3	37.3	-38.1	0	12	4	24.5	23.4
-3	1	2	62.5	-63.2	6	3	3	28.8	-30.1	2	12	4	39.4	37.4
-5	1	2	18.3	-19.0	6	3	3	61.2	-61.8	4	12	4	20.3	20.5
-7	1	2	8.2	8.3	6	3	3	63.3	-64.0	-3	11	4	7.4	-7.3
-8	0	2	8.5	8.1	6	3	3	18.5	-18.6	-5	11	4	13.3	-14.8
-6	0	2	72.1	71.2	5	3	3	11.4	-11.7	-4	10	4	10.7	11.3
-4	0	2	91.8	93.6	5	3	3	52.7	-52.6	0	10	4	7.4	-7.2
-2	0	2	36.3	-35.7	5	3	3	41.0	-42.1	2	10	4	7.0	-7.7
0	0	2	15.6	-13.5	5	3	3	14.0	-13.7	5	9	4	10.2	10.3
2	0	2	100.4	102.5	5	3	3	7.4	-7.4	3	9	4	21.9	-20.3
4	0	2	22.8	22.9	5	3	3	6.9	6.7	-1	9	4	8.4	8.6
6	0	2	30.3	29.7	4	3	3	12.0	-11.6	-3	9	4	14.9	15.0
8	0	2	34.2	35.0	4	3	3	11.8	-11.8	-5	9	4	24.4	25.1
-7	3	2	17.4	-19.3	4	3	3	13.5	-13.8	-8	8	4	18.0	18.6
-4	12	2	20.9	21.8	4	3	3	43.8	44.4	-4	8	4	9.5	10.4
-1	13	2	6.8	-6.7	4	3	3	22.2	22.5	-2	8	4	6.2	6.0
-2	14	3	7.2	7.7	4	3	3	6.5	-6.6	0	8	4	13.8	-13.3
-3	13	3	15.5	-15.6	3	3	3	34.3	-33.9	2	8	4	11.8	-11.5
-1	13	3	11.3	-11.1	3	3	3	8.5	-8.0	3	7	4	7.3	6.8
2	12	3	13.5	-12.7	-3	3	3	12.0	-12.5	-1	7	4	6.3	6.3
0	12	3	18.9	-18.0	-1	3	3	100.2	-100.9	-3	7	4	12.8	-13.0
-2	12	3	25.2	-24.8	1	3	3	79.3	-79.0	-5	7	4	25.0	-24.9
-4	12	3	28.9	-29.8	1	3	3	63.7	-64.0	-7	7	4	6.6	-7.3

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	12	0	44.6	43.8	4	0	1	24.1	-24.5	-2	8	2	8.1	8.4
1	11	0	11.2	10.9	2	0	1	72.6	-72.6	0	8	2	19.9	20.1
4	10	0	8.2	7.6	0	0	1	47.0	-49.3	2	8	2	19.3	18.9
6	10	0	7.1	6.2	-2	1	1	51.3	52.3	3	7	2	11.4	-11.0
5	9	0	23.6	21.6	-4	1	1	18.2	20.1	1	7	2	28.7	-29.8
3	9	0	26.2	27.1	-3	1	1	21.6	20.9	1	7	2	40.3	-40.8
1	9	0	20.8	-22.4	-1	1	1	16.6	18.1	-6	6	2	37.7	38.3
6	8	0	9.5	9.1	1	1	1	34.7	-34.8	-4	6	2	37.5	37.4
4	8	0	10.7	9.6	3	1	1	22.3	-22.8	0	6	2	10.7	12.4
3	7	0	6.9	-6.7	5	1	1	10.6	-10.4	2	6	2	17.1	17.9
1	7	0	23.5	25.0	6	1	1	9.5	8.9	4	6	2	22.3	21.4
4	6	0	6.6	7.7	4	1	1	17.0	16.7	6	6	2	16.4	17.4
2	6	0	83.6	84.2	2	1	1	49.9	48.8	3	5	2	25.9	-26.4
0	6	0	136.9	141.0	0	1	1	35.7	37.4	1	5	2	59.0	-58.7
5	5	0	13.6	-13.6	-2	1	1	25.5	-24.7	-1	5	2	27.3	-27.1
3	5	0	9.8	9.9	-5	1	1	34.4	-35.7	-3	5	2	15.4	-15.0
1	5	0	12.5	13.1	-3	1	1	133.2	-136.8	-4	4	2	5.6	5.9
6	4	0	20.0	18.0	-1	1	1	113.7	-114.3	-2	4	2	12.3	11.0
4	4	0	16.0	15.5	1	1	1	34.5	33.0	0	4	2	28.5	28.9
0	4	0	44.7	43.0	3	1	1	12.0	-13.2	2	4	2	48.1	49.4
7	3	0	16.4	16.0	5	1	1	20.1	-18.0	3	3	2	28.3	29.2
5	3	0	50.4	48.9	7	1	1	7.4	-7.4	1	3	2	42.3	41.3
3	3	0	46.8	48.7	4	1	1	44.4	44.7	-1	3	2	91.6	90.9
1	3	0	46.7	-44.5	-2	1	1	34.5	33.8	-3	3	2	45.5	47.6
6	2	0	11.0	9.9	-2	1	1	40.4	40.5	5	3	2	18.5	-20.3
4	2	0	27.0	27.3	-4	1	1	11.6	-13.1	1	2	2	18.0	-19.6
2	2	0	49.0	39.7	-3	1	1	19.6	20.0	-2	2	2	35.5	36.3
0	2	0	35.0	-36.7	-1	1	1	13.9	12.6	0	2	2	81.3	80.0
7	1	0	8.8	-8.1	1	1	1	35.4	-37.5	1	2	2	9.0	9.0
5	1	0	14.6	-14.5	3	1	1	36.7	-37.2	1	1	2	32.1	-32.5
3	1	0	4.5	5.6	5	1	1	16.9	-16.5	1	1	2	86.2	-83.5
1	1	0	26.8	28.7	6	1	1	11.1	-11.6	-1	1	2	59.5	-61.0
6	0	0	8.5	9.0	4	1	1	55.1	-54.0	-3	1	2	16.2	-16.1
2	0	0	108.5	109.9	2	1	1	88.7	-90.2	-6	0	2	45.8	47.5
4	12	1	12.5	-12.1	0	0	0	58.6	-52.6	-4	0	2	61.2	61.4
2	12	1	23.0	-23.5	-2	0	0	41.3	42.6	-2	0	2	34.3	-32.4
3	11	1	11.6	-11.4	-4	0	0	48.2	49.1	0	0	2	11.0	-10.2
4	10	1	11.7	10.0	-0	0	0	17.0	-15.0	0	0	2	102.0	101.6
2	10	1	13.6	13.6	-5	0	0	23.7	-22.4	4	0	2	20.6	18.9
-3	9	1	53.7	-53.5	1	0	0	10.6	-10.4	0	0	2	22.1	21.4
-1	9	1	38.9	-39.9	-4	0	0	16.0	14.7	0	0	2	19.4	17.6
1	9	1	8.0	-8.5	1	1	2	14.2	-13.9	-3	13	3	11.3	-10.5
4	8	1	14.6	13.6	-1	1	2	18.8	-18.6	0	13	3	6.1	-6.4
2	8	1	23.0	23.4	-2	1	2	7.6	7.9	0	12	3	14.4	-14.6
0	8	1	12.0	11.9	0	1	2	17.9	17.9	-2	12	3	19.8	-19.8
-2	8	1	8.3	-8.7	2	1	2	10.7	11.0	-4	12	3	19.8	-18.4
-3	7	1	9.2	8.6	3	1	2	13.0	12.2	-3	11	3	8.7	-8.6
3	7	1	26.2	-26.4	1	1	2	25.8	26.7	1	11	3	15.4	-15.2
5	7	1	13.0	-12.3	-1	1	2	53.6	53.3	1	11	3	6.7	-7.2
6	6	1	13.2	-13.0	-1	1	2	15.0	13.2	1	10	3	7.2	-6.7

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
2	10	3	6.0	-6.3	0	3	3	112.0	-108.8	-6	2	4	13.7	13.4
0	10	3	6.5	6.1	-2	3	3	40.7	-39.7	-4	2	4	29.0	29.9
-2	10	3	12.1	11.1	-1	3	3	69.5	-69.5	-2	2	4	22.2	-21.8
-4	10	3	6.7	6.7	-6	3	3	23.2	-24.7	4	2	4	8.2	-8.2
-3	9	3	8.5	-8.5	-5	3	3	11.1	-10.5	6	2	4	9.6	9.9
-1	9	3	18.7	-18.5	1	3	3	6.1	6.8	5	1	4	7.8	-8.0
1	9	3	21.8	-22.6	-2	4	4	9.5	9.2	1	1	4	8.4	8.6
3	9	3	35.1	-36.0	0	4	4	20.6	20.4	-1	1	4	15.4	-14.6
5	9	3	26.4	-25.3	2	4	4	27.9	27.3	-3	1	4	30.1	-29.9
4	8	3	8.2	-7.1	4	4	4	14.2	12.4	-5	1	4	21.3	-21.9
0	8	3	4.6	5.1	-5	4	4	9.1	-9.0	-7	1	4	9.5	-8.5
-2	8	3	20.4	21.5	0	4	4	6.2	-6.1	-4	0	4	17.7	17.4
-4	8	3	10.9	10.6	2	4	4	5.4	-5.9	-2	0	4	79.5	77.5
-5	7	3	10.9	-11.8	5	4	4	8.3	7.3	0	0	4	56.6	54.1
-3	7	3	20.4	-20.7	3	4	4	15.2	-15.2	2	0	4	117.6	116.0
-1	7	3	39.6	-39.8	-1	4	4	6.2	6.3	4	0	4	66.8	65.0
1	7	3	21.2	-20.8	-3	4	4	12.8	13.0	-4	10	4	9.5	8.7
3	7	3	9.3	9.1	-5	4	4	10.0	10.4	2	2	5	6.3	-7.7
6	6	3	10.2	8.8	-6	4	4	6.9	6.6	0	12	5	10.9	9.9
2	6	3	32.6	-33.8	-4	4	4	9.2	7.9	-1	11	5	10.8	11.2
0	6	3	29.8	-29.7	0	4	4	11.4	-11.3	4	10	5	7.5	8.4
-2	6	3	67.7	-67.4	1	4	4	10.3	-10.4	2	10	5	7.6	7.5
-4	6	3	49.3	-50.2	-1	4	4	6.0	8.5	-5	9	5	8.4	-8.0
-5	5	3	9.0	-8.4	-3	4	4	11.4	-11.1	-3	9	5	22.9	-23.6
-3	5	3	45.7	-45.9	-5	4	4	16.3	-17.4	-1	9	5	59.4	-59.4
-1	5	3	40.7	-41.1	-4	4	4	18.9	18.5	1	9	5	33.6	-32.9
1	5	3	13.5	-13.4	-2	4	4	21.1	20.8	3	9	5	7.0	6.9
3	5	3	6.3	-5.6	0	4	4	61.2	60.4	6	8	5	6.9	6.3
6	4	3	7.5	-7.4	2	4	4	85.8	84.9	4	8	5	14.1	14.4
4	4	3	10.1	-9.7	4	4	4	31.5	31.4	2	8	5	7.7	7.7
0	4	3	13.3	-12.6	5	4	4	7.6	-7.5	-1	7	5	20.8	19.8
-2	4	3	41.7	43.1	1	4	4	18.2	18.3	3	7	5	14.0	-14.2
-4	4	3	18.5	18.1	-1	4	4	14.1	-12.9	6	6	5	14.4	-14.3
-3	3	3	10.8	-11.8	-3	4	4	23.9	-23.8	4	6	5	42.8	-42.4
-1	3	3	99.9	-100.8	-5	4	4	14.2	-13.7	2	6	5	13.5	-12.8
1	3	3	78.2	-78.4	-7	4	4	8.8	-8.0	0	6	5	30.0	30.3
3	3	3	58.2	-57.8	-6	4	4	10.3	10.4	-2	0	5	13.2	14.4
5	3	3	56.8	-55.3	-4	4	4	12.0	12.1	-6	8	5	12.1	-12.6
7	3	3	19.2	-17.2	-2	4	4	23.6	24.2	-7	5	5	8.1	-7.0
4	2	3	19.3	-18.9	0	4	4	21.2	-21.8	-3	5	5	15.0	14.9
2	2	3	25.7	-25.8	2	4	4	17.9	-17.9	1	5	5	6.2	5.5
0	2	3	61.1	59.7	4	4	4	8.6	9.5	3	5	5	8.0	-8.4
-2	2	3	15.9	16.0	7	3	4	19.4	19.1	5	5	5	13.1	-13.4
-4	2	3	13.6	13.8	5	3	4	17.1	17.3	6	4	5	10.0	10.2
-5	1	3	14.8	-14.3	3	1	4	29.5	-29.5	4	4	5	24.1	23.9
-3	1	3	56.1	-57.3	1	1	4	35.6	-33.6	2	4	5	6.5	6.7
-1	1	3	78.1	-76.6	-1	1	4	44.3	46.3	0	4	5	15.6	16.7
1	1	3	38.5	-36.7	-3	1	4	28.1	28.6	-4	4	5	9.8	-9.3
4	0	3	12.9	13.3	-5	1	4	24.1	24.0	-6	4	5	0.7	9.4
6	0	3	44.2	-46.1	-7	1	4	21.3	20.2	-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/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
2	14	-3	7.7	8.1	3	-3	97.3	-98.5	-4	0	-2	23.4	23.2	
3	13	-3	14.2	-13.6	3	-3	80.6	-81.4	-6	0	-2	28.8	28.6	
1	13	-3	11.4	-10.7	3	-3	66.5	-68.3	-8	0	-2	29.7	29.9	
0	12	-3	17.2	-17.4	3	-3	71.2	-71.5	-8	2	-2	8.2	-7.8	
2	12	-3	25.8	-24.3	3	-3	27.5	-28.0	6	4	-2	14.0	-13.6	
4	12	-3	26.8	-27.5	3	-3	23.7	-24.1	2	4	-2	12.6	13.8	
3	11	-3	12.2	-11.9	3	-3	26.7	-27.8	0	4	-2	31.8	33.9	
1	11	-3	19.6	-18.6	3	-3	62.7	62.3	-2	4	-2	51.6	53.4	
-1	11	-3	8.2	-7.5	3	-3	20.1	21.0	-6	4	-2	10.4	-10.1	
-3	11	-3	8.4	7.8	3	-3	17.3	18.2	-3	5	-2	29.4	-30.0	
-4	10	-3	9.6	-8.9	3	-3	7.1	6.2	-1	5	-2	62.3	-64.0	
-2	10	-3	8.8	-8.1	3	-3	7.4	-8.3	1	5	-2	29.7	-31.7	
0	10	-3	7.0	7.4	3	-3	18.5	-18.3	3	5	-2	15.9	-18.0	
2	10	-3	14.9	15.1	3	-3	64.0	-65.7	5	5	-2	6.1	6.3	
4	10	-3	9.5	9.3	3	-3	80.0	-81.4	7	5	-2	8.3	8.4	
3	9	-3	8.0	-7.5	3	-3	39.3	-39.2	6	6	-2	54.8	56.6	
1	9	-3	20.9	-20.0	3	-3	6.0	5.9	4	6	-2	46.7	46.5	
-1	9	-3	25.9	-24.8	3	-3	8.6	-8.8	0	6	-2	6.7	6.1	
-3	9	-3	44.4	-42.6	3	-3	9.8	10.3	-2	6	-2	17.7	16.0	
-5	9	-3	37.9	-36.9	3	-3	18.6	19.4	-4	6	-2	25.9	25.0	
-4	8	-3	11.5	-10.7	3	-3	42.6	-43.8	-6	6	-2	23.8	23.4	
-2	8	-3	5.3	-5.1	3	-3	112.7	-112.4	-3	7	-2	12.8	-13.0	
0	8	-3	6.5	6.6	3	-3	49.1	-48.9	-1	7	-2	33.2	-34.7	
2	8	-3	25.5	25.8	3	-3	82.1	-83.3	1	7	-2	44.5	-46.2	
4	8	-3	13.8	13.6	3	-3	34.3	-33.4	5	7	-2	18.0	19.3	
5	7	-3	14.2	-14.3	3	-3	7.9	-7.4	6	8	-2	9.3	-9.5	
3	7	-3	24.7	-25.1	3	-3	9.1	8.7	8	8	-2	10.2	10.4	
1	7	-3	43.0	-43.6	3	-3	32.0	33.6	0	8	-2	24.7	25.1	
-1	7	-3	22.0	-22.1	3	-3	48.3	48.8	-2	8	-2	22.3	22.3	
-3	7	-3	11.2	11.5	3	-3	98.1	97.7	-6	8	-2	7.1	-8.6	
-6	6	-3	14.8	14.6	3	-3	50.4	51.3	-3	9	-2	14.8	15.0	
-4	6	-3	8.1	8.0	3	-3	29.5	-29.4	-1	9	-2	31.8	32.4	
-2	6	-3	34.9	-35.0	3	-3	7.2	-7.3	1	9	-2	63.8	63.6	
0	6	-3	31.2	-33.8	3	-3	22.4	-22.9	3	9	-2	18.3	18.4	
2	6	-3	63.8	-66.0	3	-3	40.2	42.0	2	10	-2	8.5	8.6	
4	0	-1	64.2	-63.6	3	-3	84.8	85.2	0	10	-2	20.8	20.8	
6	0	-1	18.8	-17.2	3	-3	0.2	4.7	-2	10	-2	13.8	13.0	
8	0	-1	11.2	-11.2	3	-3	10.1	9.2	-3	11	-2	7.1	-8.8	
5	5	-3	52.2	-53.6	3	-3	7.0	-7.2	-1	11	-2	18.3	-17.3	
1	5	-3	43.8	-45.4	3	-3	36.1	-36.0	1	11	-2	22.4	-21.5	
-1	5	-3	13.9	-13.8	3	-3	89.5	-89.3	-3	13	-2	6.3	-8.0	
-5	5	-3	7.2	7.2	3	-3	88.8	-87.7	-1	13	-2	14.7	-13.7	
-6	4	-3	11.0	-10.3	3	-3	16.2	-18.8	0	14	-2	7.5	7.6	
-4	4	-3	13.1	-13.1	3	-3	9.2	9.5	-2	14	-2	5.9	6.4	
0	4	-3	10.9	-11.0	3	-3	8.4	7.9	-3	13	-1	7.2	-8.2	
2	4	-3	47.1	-48.9	3	-3	70.3	68.9	-4	12	-1	18.4	-15.9	
4	4	-3	23.4	23.6	3	-3	92.7	93.4	-2	12	-1	29.3	-32.4	
7	3	-3	31.2	-30.5	3	-3	41.3	-40.6	3	11	-1	9.2	9.1	
5	3	-3	5.6	-5.7	3	-3	21.7	-19.5	-3	11	-1	15.5	-15.1	
3	3	-3	6.7	-6.3	3	-3	97.4	98.4	-5	11	-1	7.7	-7.9	

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-4	10	-1	15.2	14.8	-3	-1	42.4	-44.5	5	9	1	8.8	-7.5	
-2	10	-1	17.1	16.7	-3	-1	21.2	-21.4	7	1	2	6.1	5.3	
2	10	-1	6.9	-7.0	-3	-1	16.1	-16.2	7	7	2	6.2	5.4	
3	9	-1	69.6	-68.4	-4	0	63.7	-65.5	3	9	2	11.9	11.7	
1	9	-1	45.8	-46.4	-2	0	98.8	-98.0	4	12	2	7.7	7.6	
-1	9	-1	5.2	-6.0	0	0	51.7	-51.7	2	12	3	11.6	-11.4	
-3	9	-1	5.6	6.3	2	0	57.1	55.2	2	4	3	4.0	-4.5	
-6	8	-1	7.3	7.1	4	0	62.6	61.9	-7	3	4	32.6	32.6	
-4	8	-1	18.3	18.3	0	0	16.4	-18.4	-5	3	4	33.0	32.3	
-2	8	-1	26.9	27.0	0	0	27.0	-27.6	-3	3	4	32.5	34.2	
0	8	-1	12.0	11.8	7	3	24.5	24.1	-1	3	4	42.6	43.9	
2	8	-1	11.1	-11.8	0	3	64.4	63.6	1	3	4	43.6	-43.9	
5	7	-1	10.9	10.9	3	3	58.7	51.1	3	3	4	36.7	-37.3	
3	7	-1	11.9	12.2	1	3	57.4	-55.3	5	3	4	21.5	21.6	
-3	7	-1	31.1	-31.2	0	3	10.0	10.1	7	3	4	31.3	32.2	
-5	7	-1	17.3	-16.8	0	3	15.9	16.0	8	2	4	13.3	13.3	
-8	6	-1	17.6	-17.3	4	3	32.6	33.1	4	2	4	9.6	-9.6	
-4	6	-1	31.8	-32.2	4	3	38.1	39.3	-2	2	4	22.0	-22.9	
-2	6	-1	81.4	-83.8	0	3	42.4	-41.4	-4	2	4	34.9	35.2	
0	6	-1	49.0	-51.2	7	1	12.9	-13.0	-6	2	4	20.2	19.4	
2	6	-1	60.4	61.5	0	3	18.9	-19.2	-7	1	4	13.5	-13.2	
4	6	-1	29.5	29.4	0	3	5.8	5.8	-5	1	4	29.6	-29.6	
6	6	-1	16.6	-16.9	1	3	35.8	35.0	-3	1	4	34.5	-34.7	
3	5	-1	25.3	27.0	0	3	6.3	6.9	-1	1	4	16.7	-16.3	
1	5	-1	20.1	20.9	0	3	8.0	7.4	1	1	4	11.4	11.2	
-1	5	-1	37.8	-39.7	0	3	119.4	119.5	5	1	4	9.9	-9.5	
-3	5	-1	27.8	-29.2	0	3	6.3	6.5	7	1	4	9.6	-9.0	
-5	5	-1	14.5	-14.2	0	3	25.7	24.7	6	0	4	8.7	-8.1	
-8	4	-1	12.1	11.7	4	4	18.8	18.8	4	0	4	78.6	77.7	
-4	4	-1	22.5	22.6	0	4	37.4	38.7	2	0	4	127.0	126.7	
-2	4	-1	53.5	55.7	7	7	11.8	-11.7	0	0	4	84.2	81.5	
0	4	-1	38.4	40.1	0	4	17.6	-17.6	-2	0	4	82.2	81.5	
2	4	-1	27.4	-28.5	0	4	10.7	10.9	-4	0	4	18.3	17.1	
5	3	-1	47.1	-46.7	3	3	16.7	18.0	-8	0	4	6.4	-6.1	
3	3	-1	153.3	-153.9	0	4	90.9	93.5	0	4	4	7.5	7.5	
-1	3	-1	119.1	-119.2	1	2	152.2	153.4	4	4	4	9.8	9.4	
-1	3	-1	40.8	40.5	7	7	6.2	-7.3	2	4	4	22.1	-21.8	
-3	3	-1	6.5	-6.0	0	7	9.1	-8.9	0	4	4	23.7	-24.9	
-5	3	-1	21.0	-20.8	3	3	6.6	-8.9	-2	4	4	25.3	25.2	
-7	3	-1	10.5	-10.6	1	7	27.2	28.9	-4	4	4	16.4	16.3	
-6	2	-1	6.4	6.8	0	7	14.1	13.9	-6	4	4	15.7	15.0	
-4	2	-1	51.9	52.3	4	4	12.7	12.3	-7	5	4	10.4	-12.0	
-2	2	-1	38.7	40.2	0	7	4.8	-4.2	-5	5	4	19.8	-19.8	
0	2	-1	10.4	10.6	0	7	31.0	32.4	-3	5	4	28.0	-27.8	
2	2	-1	37.3	38.2	0	7	34.0	33.0	-1	5	4	13.1	-13.0	
4	2	-1	16.1	-17.1	0	7	28.9	-29.4	1	5	4	21.8	22.6	
5	1	-1	6.7	7.0	0	7	10.0	9.8	5	5	4	10.2	-9.5	
3	1	-1	26.4	27.4	0	7	7.4	-7.5	7	5	4	7.6	-7.0	
1	1	-1	16.9	16.0	0	7	14.5	13.8	4	6	4	41.0	41.0	
-1	1	-1	40.6	-41.5	0	7	55.4	56.0	2	6	4	95.2	97.2	

Sample 9. 1pq16-4A (continued)

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	4	9	25.4	-25.8	4	6	10	13.6	-13.1	0	0	11	45.6	-44.3
4	4	9	9.7	9.6	0	6	10	32.5	33.1	2	0	11	44.4	-42.8
3	3	9	33.7	-33.0	-2	6	10	32.3	32.1	4	0	11	8.4	8.5
-1	3	9	64.8	-62.7	-4	6	10	33.7	34.1	-1	3	11	5.5	4.2
-3	3	9	71.0	-70.5	-6	6	10	22.9	23.1	-5	3	12	14.0	14.7
-5	3	9	61.8	-60.4	-3	7	10	7.7	7.1	-3	3	12	43.3	43.0
-7	3	9	24.1	-23.0	-1	7	10	16.2	-16.0	-1	3	12	44.6	43.1
-6	2	9	9.8	9.5	3	7	10	9.9	-10.1	3	3	12	17.3	-18.0
-2	2	9	16.9	17.3	1	7	10	8.6	9.1	0	2	12	7.1	7.2
6	2	9	26.8	-26.1	4	8	10	8.5	9.1	-2	2	12	29.3	29.2
5	1	9	9.7	9.7	2	8	10	10.4	-10.0	-4	2	12	16.3	17.1
3	1	9	11.7	-12.4	-4	8	10	14.4	14.8	-5	1	12	7.4	-7.8
-1	1	9	15.5	-15.2	1	9	10	23.1	24.1	-3	1	12	13.8	-13.6
-5	1	9	7.8	6.5	3	9	10	7.6	7.1	-1	1	12	14.1	-13.1
-7	1	9	15.1	-15.8	1	10	10	6.8	7.1	3	1	12	10.4	10.5
-6	0	9	13.0	-13.0	-4	10	10	7.9	-8.1	4	0	12	26.9	28.2
-2	0	9	37.9	-37.6	-2	10	11	7.3	7.1	2	0	12	51.1	50.6
4	0	9	17.4	17.8	0	10	11	9.9	10.1	0	0	12	32.6	30.9
6	0	9	20.1	-19.2	-1	9	11	12.9	13.1	-2	0	12	19.7	-19.0
-5	0	9	14.3	-12.0	-3	9	11	14.6	-14.1	-6	0	12	21.8	24.0
3	0	9	28.5	-29.7	-2	8	11	11.0	11.1	-2	4	12	18.8	19.3
1	3	10	11.0	-10.6	0	8	11	14.7	16.0	-4	4	12	14.8	15.8
3	3	10	14.7	13.6	2	8	11	8.9	9.1	-6	4	12	13.3	14.3
5	3	10	42.5	42.0	3	7	11	6.4	-6.1	-5	5	12	8.0	7.9
4	2	10	23.4	25.1	1	7	11	11.2	-12.1	-3	5	12	7.8	-7.9
2	2	10	8.3	8.3	-1	7	11	7.2	-7.1	-1	5	12	7.7	-8.2
0	2	10	24.0	24.0	-3	7	11	8.0	-8.1	3	5	12	10.3	-11.4
-2	2	10	15.9	14.6	-2	6	11	13.3	-13.1	-1	5	12	10.3	11.0
-4	2	10	15.3	-15.8	0	6	11	41.0	-42.1	2	6	12	39.2	40.6
-3	1	10	7.2	6.9	2	6	11	23.5	-24.1	0	6	12	11.6	11.9
-1	1	10	9.8	-8.9	1	5	11	12.5	-13.1	-2	6	12	7.3	-7.7
1	1	10	19.0	-17.7	-1	5	11	18.4	-19.1	-3	7	12	12.5	-12.9
3	1	10	18.2	-17.7	0	4	11	18.3	18.1	-1	7	12	6.1	-7.1
5	1	10	8.5	-8.0	2	4	11	27.7	28.1	0	8	12	9.6	9.9
4	0	10	8.4	-7.6	1	3	11	10.5	10.1	-2	8	12	12.0	11.7
0	0	10	43.3	41.9	2	3	11	24.4	-25.1	-4	8	12	9.1	9.0
-2	0	10	64.9	63.7	3	3	11	11.5	-11.1	-3	9	12	29.8	30.8
-4	0	10	35.6	36.4	3	3	11	19.8	18.1	-1	9	12	22.6	23.3
-6	0	10	29.8	30.5	-1	3	11	34.3	-33.1	-2	10	12	9.0	9.9
4	4	10	16.3	16.0	-3	3	11	28.4	-27.1	-1	1	13	23.3	-26.0
2	4	10	12.0	12.0	-5	3	11	15.2	-16.1	1	7	13	8.3	9.8
0	4	10	8.3	8.1	-6	2	11	8.4	-8.1	-4	6	13	23.7	-23.7
-4	4	10	15.8	-15.7	-4	2	11	10.7	11.1	-2	6	13	7.6	8.0
-5	5	10	9.3	8.0	-2	2	11	17.6	17.1	0	6	13	17.3	18.0
-1	5	10	10.2	-10.0	0	2	11	21.0	19.1	-1	5	13	7.2	7.7
1	5	10	10.7	-9.9	2	2	11	20.0	20.1	-0	5	13	9.0	-10.0
3	5	10	14.6	-14.9	3	1	11	5.3	-4.1	-4	4	13	13.0	14.0
5	5	10	8.7	-8.7	1	1	11	18.6	-17.1	0	4	13	6.1	-6.2
					-1	1	11	21.1	-19.1	3	3	13	9.2	-10.6
					-2	0	11	15.1	-13.1	1	3	13	30.0	-30.5

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-1	3	13	52.0	-51.3	-2	2	14	9.4	-9.1	1	3	15	7.6	-8.3
-3	3	13	12.4	-12.3	-4	2	14	8.8	-8.1	-1	3	15	7.6	-8.0
-5	3	13	13.5	13.0	1	1	14	8.8	-8.1	-3	3	15	9.6	-11.0
-6	2	13	8.8	9.2	3	1	14	11.3	-11.1	-4	2	15	5.9	-6.2
-4	2	13	7.3	7.7	0	1	14	7.6	-7.1	0	2	15	13.0	14.4
-2	2	13	9.7	10.3	2	0	14	7.7	-7.1	1	1	15	12.0	-12.8
0	2	13	9.2	-8.9	-2	0	14	35.9	36.0	-1	1	15	12.8	-13.5
1	1	13	7.8	7.7	-4	0	14	40.9	41.0	-2	0	15	12.4	-11.9
-3	1	13	7.7	-7.5	2	4	14	9.6	10.3	0	0	15	20.1	-21.9
-5	1	13	10.2	-11.0	1	3	14	9.3	-10.0	2	8	15	14.6	-15.6
-6	0	13	24.0	-25.7	0	5	14	7.5	-7.6	-1	3	16	14.7	16.3
-4	0	13	24.5	-24.6	1	6	14	10.1	10.0	0	2	16	6.5	6.4
0	0	13	28.2	27.0	0	6	14	25.8	26.9	-3	1	16	9.5	-10.6
4	0	13	13.9	-15.3	-2	6	14	23.0	20.4	-1	1	16	8.9	-9.7
-3	3	14	17.8	-18.4	-4	6	14	14.1	-15.5	-2	0	16	7.4	8.4
1	3	14	11.7	11.8	-2	6	15	14.1	-15.5					
					-1	5	15	10.2	-10.7					

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-1	7	8	18.7	-20.0	-1	7	-7	8.3	-8.5	-1	7	-7	8.3	-8.5
-1	7	12	8.4	-8.1	-1	7	-6	14.9	-14.5	-1	7	-6	14.9	-14.5
-1	9	-1	-8.1	-8.5	-1	7	-3	28.1	-26.1	-1	7	-3	28.1	-26.1
-1	9	0	31.4	-31.6	-1	7	-2	38.2	-36.4	-1	7	-2	38.2	-36.4
-1	9	0	48.5	-50.4	-1	5	-14	11.4	-11.5	-1	5	-14	11.4	-11.5
-1	9	0	78.4	71.1	-1	5	-11	13.5	-14.2	-1	5	-11	13.5	-14.2
-1	9	0	25.7	-26.5	-1	5	-10	12.0	-12.5	-1	5	-10	12.0	-12.5
-1	9	0	8.4	9.1	-1	5	-7	29.4	-30.1	-1	5	-7	29.4	-30.1
-1	9	0	82.5	-83.2	-1	5	-6	32.9	-33.8	-1	5	-6	32.9	-33.8
-1	9	0	25.3	25.4	-1	5	-4	20.3	20.5	-1	5	-4	20.3	20.5
-1	9	0	24.1	25.5	-1	5	-3	16.2	-15.8	-1	5	-3	16.2	-15.8
-1	9	0	40.1	-40.4	-1	5	-2	64.8	-65.2	-1	5	-2	64.8	-65.2
-1	0	10	6.7	-6.7	-1	3	-15	12.6	-12.0	-1	3	-15	12.6	-12.0
-1	0	10	31.2	32.1	-1	3	-14	17.3	16.1	-1	3	-14	17.3	16.1
-1	0	10	36.4	-34.9	-1	3	-13	41.5	-43.1	-1	3	-13	41.5	-43.1
-1	0	10	16.9	17.4	-1	3	-11	19.7	20.1	-1	3	-11	19.7	20.1
-1	0	10	28.0	-27.9	-1	3	-10	13.7	13.9	-1	3	-10	13.7	13.9
-1	0	10	24.3	-24.4	-1	3	-9	67.0	-67.4	-1	3	-9	67.0	-67.4
-1	0	10	17.3	17.6	-1	3	-8	16.4	-17.0	-1	3	-8	16.4	-17.0
-1	0	10	19.5	-20.3	-1	3	-7	37.2	-36.4	-1	3	-7	37.2	-36.4
-1	0	10	11.7	-11.5	-1	3	-6	125.9	129.5	-1	3	-6	125.9	129.5
-1	0	10	11.1	-11.7	-1	3	-4	39.6	-38.8	-1	3	-4	39.6	-38.8
-1	0	10	9.9	9.7	-1	3	-3	65.3	-64.4	-1	3	-3	65.3	-64.4
-1	0	10	8.1	8.0	-1	3	-2	40.5	39.2	-1	3	-2	40.5	39.2
-1	0	10	8.4	-8.5	-1	1	-15	16.8	-16.2	-1	1	-15	16.8	-16.2
-1	0	10	14.8	-14.3	-1	1	-14	13.7	-12.6	-1	1	-14	13.7	-12.6
-1	0	10	10.0	-10.1	-1	1	-13	9.2	9.3	-1	1	-13	9.2	9.3
-1	0	10	11.3	-11.3	-1	1	-11	18.2	-18.6	-1	1	-11	18.2	-18.6
-1	0	10	11.1	-11.2	-1	1	-10	20.0	-20.8	-1	1	-10	20.0	-20.8
-1	0	10	11.9	11.6	-1	1	-7	30.0	-30.3	-1	1	-7	30.0	-30.3
-1	0	10	18.2	-19.0	-1	1	-6	34.3	-33.9	-1	1	-6	34.3	-33.9
-1	0	10	12.4	-13.8	-1	1	-3	40.2	-41.4	-1	1	-3	40.2	-41.4
-1	0	10	10.0	-10.0	-1	1	-2	86.9	-84.4	-1	1	-2	86.9	-84.4
-1	0	10	11.4	-11.3	0	14	4	7.4	-7.7	0	14	4	7.4	-7.7
-1	0	10	21.6	-20.7	0	14	2	9.0	10.0	0	14	2	9.0	10.0
-1	0	10	17.4	17.5	0	12	8	31.9	31.5	0	12	8	31.9	31.5
-1	0	10	19.0	18.4	0	12	7	28.2	-27.9	0	12	7	28.2	-27.9
-1	0	10	31.4	-32.8	0	12	5	19.0	19.1	0	12	5	19.0	19.1
-1	0	10	13.4	-13.6	0	12	4	28.3	29.3	0	12	4	28.3	29.3
-1	0	10	31.3	-30.0	0	12	3	21.1	-21.8	0	12	3	21.1	-21.8
-1	0	10	45.7	-46.6	0	12	1	19.7	-20.3	0	12	1	19.7	-20.3
-1	0	10	7.9	-7.0	0	12	0	69.7	70.0	0	12	0	69.7	70.0
-1	0	10	29.7	-29.6	0	10	12	8.5	8.0	0	10	12	8.5	8.0
-1	0	10	30.2	31.9	0	10	11	13.3	14.2	0	10	11	13.3	14.2
-1	0	10	13.1	13.3	0	10	10	6.2	6.4	0	10	10	6.2	6.4
-1	0	10	14.0	-14.9	0	10	9	10.7	-10.0	0	10	9	10.7	-10.0
-1	0	10	20.2	-21.1	0	10	7	18.1	18.9	0	10	7	18.1	18.9
-1	0	10	7.7	-8.0	0	10	6	19.2	19.1	0	10	6	19.2	19.1
-1	0	10	8.2	7.9	0	10	4	8.1	-8.5	0	10	4	8.1	-8.5
-1	0	10			0	10	3	8.1	8.5	0	10	3	8.1	8.5

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	10	2	23.6	23.8	0	2	0	34.1	-36.6	2	6	3	40.5	-41.9
0	10	0	6.4	-8.0	0	2	15	28.2	-27.7	2	6	2	21.5	22.0
0	8	12	12.2	13.2	0	0	13	33.3	32.7	2	6	1	86.2	-86.0
0	8	11	20.0	20.6	0	0	12	40.1	38.2	2	6	0	99.9	100.6
0	8	9	14.7	-15.6	0	0	11	47.7	-48.4	2	6	-1	64.2	85.1
0	8	8	8.9	-8.8	0	0	10	44.6	45.1	2	4	14	15.3	13.8
0	8	7	29.0	29.3	0	0	9	23.7	-26.2	2	4	11	12.9	12.6
0	8	6	31.3	31.1	0	0	8	74.0	74.4	2	4	10	15.4	14.2
0	8	4	15.2	-15.4	0	0	7	57.5	-57.6	2	4	7	19.1	19.0
0	8	2	26.0	25.9	0	0	6	39.6	39.9	2	4	6	40.4	39.7
0	8	1	14.5	14.8	0	0	5	102.4	102.2	2	4	5	8.1	8.1
0	6	14	12.5	12.5	0	0	4	53.6	54.2	2	4	4	21.8	-20.3
0	6	13	23.0	22.8	0	0	3	107.9	-106.2	2	4	2	54.8	55.5
0	6	12	16.8	15.8	0	0	2	58.1	-53.8	2	4	1	56.1	56.6
0	6	11	50.0	-49.4	0	0	1	102.4	-104.2	2	4	0	27.5	-26.0
0	6	10	37.3	38.9	0	1	0	8.1	8.6	2	2	13	9.7	-8.9
0	6	8	66.6	68.0	2	2	14	13.1	13.0	2	2	11	32.0	30.7
0	6	7	56.9	-56.6	2	2	13	21.5	21.7	2	2	10	26.2	26.8
0	6	6	6.5	-7.6	2	2	12	11.0	-11.4	2	2	9	32.5	-32.2
0	6	5	38.1	36.0	2	2	11	14.0	-12.9	2	2	8	61.5	60.2
0	6	4	71.3	69.0	2	2	10	49.3	48.3	2	2	6	49.1	51.1
0	6	3	30.6	-31.3	2	2	9	16.3	-15.1	2	2	5	28.2	-28.4
0	6	2	11.6	13.7	2	2	8	10.7	10.4	2	2	4	40.6	39.7
0	6	1	53.1	-55.2	2	2	7	41.0	-40.5	2	2	3	48.8	45.0
0	6	0	155.1	157.9	2	2	6	39.3	39.2	2	2	2	45.0	43.7
0	4	13	6.1	-6.0	2	2	5	23.6	23.5	2	2	1	20.9	-19.8
0	4	12	24.2	23.4	2	2	4	10.7	10.1	2	2	0	61.7	61.9
0	4	11	31.9	32.0	2	2	3	11.1	-12.1	2	2	0	48.6	-48.9
0	4	10	8.8	8.5	2	2	2	26.8	26.0	2	2	0	74.0	74.2
0	4	9	26.0	-27.9	2	2	10	12.7	11.6	2	2	7	18.0	19.4
0	4	8	14.5	-14.4	2	2	9	9.7	-9.4	2	2	6	22.2	-22.9
0	4	7	44.6	46.7	2	2	8	9.6	-10.2	2	2	5	52.3	-53.1
0	4	6	59.1	61.4	2	2	7	14.6	15.2	2	2	4	128.4	128.2
0	4	5	18.0	18.7	2	2	6	21.0	20.3	2	2	3	45.7	-46.1
0	4	4	23.1	-23.4	2	2	5	10.9	11.8	2	2	2	112.1	109.9
0	4	3	14.1	-14.5	2	2	4	11.0	11.7	2	2	1	97.1	-94.7
0	4	2	30.0	31.3	2	2	3	11.5	-10.3	2	2	0	118.2	118.5
0	4	1	41.7	43.7	2	2	2	7.5	8.7	2	2	0	51.0	50.0
0	4	0	44.9	45.1	2	2	1	27.3	27.5	2	2	0	39.7	-37.1
0	2	15	18.2	18.5	2	2	0	11.5	11.0	2	2	0	41.6	-40.6
0	2	13	6.8	-10.1	2	2	0	14.4	-12.7	2	2	0	66.2	64.2
0	2	12	7.9	7.4	2	2	0	26.2	25.7	2	2	0	40.5	39.3
0	2	11	21.8	21.4	2	2	0	29.2	30.4	2	2	0	103.2	104.3
0	2	10	18.5	17.3	2	2	0	11.4	-11.6	2	2	0	127.2	-129.8
0	2	7	38.7	38.7	2	2	0	55.0	54.0	2	2	0	36.6	38.0
0	2	6	22.9	23.4	2	2	0	26.8	-27.7	2	2	0	15.7	17.0
0	2	5	8.3	-7.5	2	2	0	7.4	-6.8	2	2	0	66.3	67.6
0	2	3	62.3	59.8	2	2	0	38.3	38.7	2	2	0	13.3	-13.9
0	2	2	82.1	81.3	2	2	0	9.5	-9.1	2	2	0	21.0	-20.3
					2	2	0	14.7	-14.8	2	2	0	43.5	42.9

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

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
2	12	-1	19.1	16.4	4	8	0	13.2	12.1	-1	7	2	41.5	-42.2
0	12	-1	13.6	-13.4	1	7	0	26.9	27.8	-5	7	2	11.0	10.2
-2	12	-1	28.0	-26.4	2	6	0	84.4	85.8	-6	6	2	55.3	54.2
-3	11	-1	13.8	-12.7	0	6	0	150.2	151.8	-4	6	2	45.1	44.8
-2	10	-1	14.9	14.4	1	5	0	19.6	19.1	2	6	2	15.5	16.1
-4	10	-1	12.6	12.1	3	5	0	11.5	10.0	1	5	2	59.9	-61.3
1	9	-1	40.3	-40.6	5	5	0	19.9	-19.0	-1	5	2	28.5	-20.6
0	8	-1	9.6	8.1	6	4	0	24.3	22.9	-3	5	2	16.7	-15.3
-2	8	-1	25.0	24.3	4	4	0	18.8	18.7	-6	4	2	13.7	-14.3
-4	8	-1	18.4	17.9	0	4	0	31.3	30.1	-2	4	2	13.6	13.4
-5	7	-1	15.3	-14.9	1	3	0	60.0	-60.4	0	4	2	36.3	36.2
-3	7	-1	29.6	-29.0	3	3	0	48.2	47.8	2	4	2	48.7	51.2
2	6	-1	59.2	58.1	5	3	0	66.9	65.9	1	3	2	57.0	56.5
0	6	-1	44.2	-44.8	7	3	0	24.9	24.9	-1	3	2	95.8	95.6
-2	6	-1	78.2	-79.2	6	2	0	19.3	19.0	-3	3	2	48.4	48.0
-4	6	-1	34.8	-33.7	4	2	0	34.0	32.4	-5	3	2	34.5	-33.2
-6	6	-1	16.6	-15.1	2	2	0	30.7	32.0	-7	3	2	20.8	-21.2
-5	5	-1	13.3	-13.4	0	2	0	52.6	-49.8	-8	2	2	11.1	-12.0
-3	5	-1	28.3	-28.9	1	1	0	35.1	30.0	-4	2	2	20.4	-21.9
-1	5	-1	40.6	-40.2	5	1	0	28.2	-21.6	-2	2	2	38.7	40.0
1	5	-1	21.3	21.3	7	1	0	13.9	-13.7	0	2	2	91.8	88.9
2	4	-1	26.7	-29.7	2	0	0	119.5	122.1	2	2	2	10.6	10.0
0	4	-1	34.2	34.3	-5	9	1	28.3	-26.7	1	1	2	93.3	-91.4
-2	4	-1	54.9	54.7	-3	9	1	62.1	-62.2	-1	1	2	64.1	-66.0
-4	4	-1	25.7	26.1	-4	8	1	8.9	-8.8	-3	1	2	16.2	-19.2
-6	4	-1	11.8	9.6	-5	7	1	10.9	9.2	-8	0	2	24.0	22.0
-5	3	-1	16.3	-17.4	-3	7	1	12.0	11.9	-6	0	2	73.9	73.2
-1	3	-1	49.7	46.8	-4	6	1	33.8	31.8	-4	0	2	86.6	89.5
1	3	-1	125.6	-123.9	-6	6	1	18.5	-17.2	-2	0	2	43.6	-43.8
2	2	-1	27.5	28.9	-3	5	1	26.5	27.0	0	0	2	39.3	-33.0
-2	2	-1	40.9	43.0	-5	3	1	50.5	-49.0	2	0	2	92.9	90.7
-4	2	-1	50.7	50.7	-3	3	1	158.9	-160.8	-2	12	3	18.1	-18.5
-5	1	-1	20.3	-20.7	-4	2	1	20.5	-21.3	-4	12	3	21.9	-21.0
-3	1	-1	42.2	-44.8	-3	1	1	27.1	28.2	-1	11	3	14.9	-14.1
-1	1	-1	41.3	-41.6	-4	0	1	63.4	63.2	-2	10	3	13.9	14.4
1	1	-1	16.8	16.8	-6	0	1	20.4	-21.1	-1	9	3	14.7	-13.7
2	0	-1	56.2	57.2	-0	0	1	30.0	-30.0	1	9	3	10.1	-10.9
0	0	-1	43.1	-40.8	-4	12	2	18.4	18.2	0	8	3	0.2	0.0
-2	0	-1	102.0	-100.6	1	11	2	13.8	-13.7	-2	8	3	21.8	22.1
-4	0	-1	65.6	-64.8	-1	11	2	15.3	-16.2	-4	8	3	12.5	12.7
-6	0	-1	17.5	-18.0	0	10	2	17.4	17.6	-5	7	3	12.3	-12.3
2	0	-1	11.6	-11.8	2	10	2	15.2	14.1	-3	7	3	23.0	-22.6
2	10	-1	9.8	-9.0	1	9	2	30.6	29.6	-1	7	3	37.8	-39.1
2	12	0	25.3	23.2	-1	9	2	55.5	55.1	1	7	3	18.6	-18.5
0	12	0	45.3	43.1	3	9	2	16.7	15.8	2	6	3	27.7	-30.1
1	11	0	10.8	11.8	-5	9	2	19.3	-17.9	0	6	3	35.7	-34.3
1	9	0	29.6	-29.6	-2	8	2	11.3	10.6	-2	6	3	59.5	-59.2
3	9	0	27.5	26.6	0	8	2	25.2	25.0	-4	6	3	58.1	-58.0
5	9	0	30.0	30.4	2	8	2	18.5	18.7	-6	6	3	18.0	-16.5
6	8	0	12.2	12.6	1	7	2	31.2	-31.7	-5	5	3	12.2	-10.4

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-3	5	3	49.4	-49.5	-2	2	4	18.2	-18.4	2	6	6	16.6	-18.3
-1	5	3	40.7	-42.1	1	1	4	13.2	15.3	1	5	6	29.3	-31.7
1	5	3	11.0	-11.3	-1	1	4	13.3	-12.2	-3	5	6	18.6	18.9
-2	4	3	47.9	47.6	-3	1	4	30.1	-31.0	-5	5	6	9.5	9.1
-4	4	3	25.1	23.9	-5	1	4	25.7	-26.7	-4	4	6	10.1	-10.1
-7	3	3	29.7	-28.9	-7	1	4	12.4	-12.2	0	4	6	49.1	50.0
-1	3	3	84.7	-85.6	-4	0	4	14.9	15.0	2	4	6	36.7	38.7
1	3	3	77.6	-78.4	-2	0	4	77.5	77.0	1	3	6	125.8	126.4
2	2	3	25.8	-27.6	0	0	4	64.6	65.0	-1	3	6	44.4	46.2
0	2	3	63.1	62.5	2	0	4	131.5	138.2	-3	3	6	38.7	-41.4
-2	2	3	24.3	24.7	-1	11	5	9.5	10.0	-2	2	6	23.5	24.6
-4	2	3	18.5	20.2	-3	9	5	26.1	-24.7	0	2	6	23.1	24.4
-5	1	3	17.5	-17.4	-1	9	5	59.7	-61.3	2	2	6	52.1	54.7
-3	1	3	61.3	-63.6	1	9	5	34.2	-36.4	1	1	6	33.0	-34.4
-1	1	3	79.4	-80.2	-1	7	5	21.7	22.3	-1	1	6	8.9	-9.7
1	1	3	35.3	-35.2	2	6	5	16.1	-17.0	-3	1	6	16.7	16.9
2	0	3	41.5	-43.1	0	6	5	40.0	39.1	-5	1	6	12.2	13.8
0	0	3	126.3	-117.9	-2	6	5	22.3	22.0	-6	0	6	39.9	38.4
-2	0	3	51.4	-52.1	-6	6	5	16.7	-15.7	-4	0	6	93.4	95.0
-4	0	3	80.9	-82.2	-3	5	5	10.0	10.0	-2	0	6	95.7	96.2
-6	0	3	30.2	-29.7	0	4	5	0.7	0.0	0	0	6	27.6	26.6
-8	0	3	16.3	15.5	-6	4	5	11.3	10.0	2	0	6	29.7	-31.1
0	12	4	16.8	18.2	-5	3	5	22.2	-20.0	-2	12	7	23.4	-24.7
2	12	4	30.3	29.8	-3	3	5	65.7	-65.0	-5	9	7	25.0	-22.0
-3	9	4	16.0	15.7	-1	3	5	124.3	-124.4	-1	9	7	18.7	20.2
-5	9	4	19.3	20.9	1	3	5	98.7	-99.2	1	9	7	16.7	-15.9
-4	8	4	13.2	12.8	2	2	5	38.0	38.0	0	8	7	19.3	20.8
0	8	4	11.5	-11.6	0	2	5	13.0	-14.3	-2	8	7	16.8	18.5
-3	7	4	11.5	-11.1	-2	2	5	16.2	-17.2	-3	7	7	15.7	-15.3
-5	7	4	18.3	-19.2	-4	2	5	10.8	10.0	-1	7	7	27.3	-28.8
-4	6	4	15.1	15.2	-3	1	5	16.5	18.0	0	6	7	49.0	-51.5
-2	6	4	22.3	21.9	-1	1	5	16.7	16.0	-2	6	7	64.0	-64.8
0	6	4	64.3	61.8	2	0	5	48.7	-47.0	-4	6	7	17.6	-18.5
2	6	4	89.0	91.5	0	0	5	107.3	107.0	-3	5	7	13.8	-15.7
1	5	4	22.7	24.5	-2	0	5	48.9	49.0	-1	5	7	25.1	-28.1
-1	5	4	10.5	-11.0	-4	0	5	27.7	-30.2	1	5	7	24.5	-25.7
-3	5	4	25.4	-24.8	-6	0	5	17.0	-17.0	2	4	7	13.1	13.8
-5	5	4	17.4	-17.1	-8	0	5	15.5	-16.0	0	4	7	38.7	39.5
-6	4	4	15.2	16.0	-4	12	6	22.0	22.0	-2	4	7	22.6	23.8
-4	4	4	20.8	19.4	-2	12	6	19.3	20.0	-4	4	7	14.5	13.6
-2	4	4	22.9	23.0	0	10	6	12.2	12.0	-7	3	7	36.2	-37.0
0	4	4	23.2	-24.3	1	9	6	48.9	49.0	-5	3	7	41.3	-40.2
2	4	4	21.0	-23.1	-1	9	6	16.4	16.0	-1	3	7	27.8	28.4
1	3	4	49.5	-49.0	-3	9	6	11.0	-12.7	1	3	7	25.4	-25.6
-1	3	4	41.1	41.0	0	8	6	18.9	19.0	0	2	7	38.3	38.9
-3	3	4	38.8	38.8	2	8	6	21.2	22.1	-2	2	7	52.2	55.0
-5	3	4	33.1	34.4	1	7	6	13.6	-13.0	-3	1	7	22.9	-23.5
-7	3	4	30.7	33.2	-6	6	6	20.5	21.0	-1	1	7	40.2	-41.5
-6	2	4	20.3	19.9	-4	6	6	64.4	64.0	1	1	7	27.3	-29.3
-4	2	4	33.4	35.1	-2	6	6	68.5	67.0	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/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
7	1	0	13.2	-13.8	-2	1	0	9.5	-9.7	-7	1	1	7.4	-7.6
5	1	0	19.9	-20.2	2	1	0	17.8	18.1	8	0	1	26.7	-26.9
3	1	0	7.4	6.7	4	1	0	14.5	13.9	-6	0	1	18.3	-17.8
1	1	0	38.1	42.6	-1	1	0	46.8	-46.4	-4	0	1	60.7	60.5
8	2	0	9.2	9.2	-3	1	0	71.3	-69.7	2	0	1	60.5	62.7
6	2	0	18.2	17.9	-5	1	0	30.5	-30.1	0	0	1	52.2	-48.6
4	2	0	32.8	33.5	-2	1	0	11.9	-11.2	1	0	1	99.2	-100.4
2	2	0	33.4	32.5	0	1	0	10.8	9.6	-1	0	1	64.8	-62.5
0	2	0	45.1	-47.5	2	1	0	26.1	25.7	8	0	1	17.1	-17.4
7	3	0	24.0	24.6	4	1	0	21.2	19.8	0	1	2	7.3	7.5
5	3	0	64.3	62.2	5	1	0	15.2	-15.8	-1	1	2	9.0	-8.5
3	3	0	47.5	48.9	3	1	0	29.8	-29.8	1	1	2	11.2	-12.5
1	3	0	60.3	-61.6	-3	1	0	12.4	11.9	-4	1	2	18.4	19.3
8	4	0	7.4	7.0	-5	1	0	9.7	9.3	1	1	2	19.6	-20.3
6	4	0	24.6	23.5	-7	1	0	6.2	-5.7	1	1	2	16.6	-16.5
4	4	0	18.7	18.9	-0	1	0	16.5	-16.3	2	1	2	14.8	15.2
0	4	0	30.6	28.6	-4	1	0	31.6	32.2	0	1	2	19.5	19.5
7	5	0	12.6	-12.2	-2	1	0	62.4	60.2	2	1	2	7.8	8.2
5	5	0	17.9	-17.9	0	1	0	49.6	-49.4	5	1	2	21.2	-20.7
3	5	0	11.0	11.9	2	1	0	81.2	-80.7	3	1	2	19.3	18.0
1	5	0	20.5	18.6	4	1	0	33.3	-32.9	1	1	2	64.2	62.5
0	6	0	92.9	90.3	8	1	0	15.8	-15.8	1	1	2	33.2	31.7
0	8	0	161.9	161.1	5	1	0	14.7	-14.0	3	1	2	13.9	15.5
5	7	0	11.8	-11.1	3	1	0	29.5	-28.8	5	1	2	10.2	9.9
3	7	0	8.1	-7.8	-1	1	0	40.6	-40.6	2	1	2	21.2	21.1
1	7	0	30.0	29.1	1	1	0	20.8	20.3	0	1	2	28.0	27.2
7	7	0	7.5	-7.9	-3	1	0	26.0	26.0	-2	1	2	11.9	12.0
6	8	0	12.6	13.2	-2	1	0	30.1	-29.4	8	1	2	10.1	-10.1
4	8	0	12.8	12.9	0	1	0	35.4	35.1	5	1	2	10.8	10.9
0	8	0	9.8	-8.0	2	1	0	55.5	55.1	1	1	2	46.5	-46.2
5	9	0	32.4	31.8	4	1	0	26.3	25.6	1	1	2	34.0	-33.4
3	9	0	31.9	30.5	6	1	0	10.5	11.5	3	1	2	12.1	-12.0
1	9	0	33.7	-31.8	7	1	0	9.0	-9.4	6	1	2	23.2	23.9
6	10	0	9.5	9.8	5	1	0	16.2	-16.7	4	1	2	21.5	22.4
4	10	0	9.3	8.7	-1	1	0	47.7	44.0	2	1	2	16.7	18.4
0	10	0	7.4	-7.4	-3	1	0	127.7	-127.9	4	1	2	49.5	48.4
1	11	0	13.5	13.6	-5	1	0	163.7	-163.0	6	1	2	58.2	56.7
2	12	0	30.0	29.2	-8	1	0	49.6	-48.4	7	1	2	8.3	8.6
0	12	0	55.5	54.0	-4	1	0	10.9	10.9	5	1	2	16.6	-16.1
1	13	0	7.8	7.6	-6	1	0	17.4	-18.0	0	1	2	28.0	-28.0
2	14	1	8.7	8.8	-2	1	1	27.4	27.2	0	1	2	62.4	-62.1
3	13	1	8.6	-8.1	2	1	1	39.0	41.1	0	1	2	28.2	-28.7
1	13	1	7.3	-7.1	4	1	1	58.0	51.5	4	1	2	7.3	-8.9
-4	12	1	15.2	14.2	6	1	1	9.3	9.3	4	1	2	51.7	52.3
-2	12	1	20.6	20.1	5	1	1	19.4	-20.9	4	1	2	37.8	38.3
0	12	1	17.3	-16.7	3	1	1	43.8	-43.3	2	1	2	13.5	12.8
2	12	1	31.4	-31.5	1	1	1	40.5	-44.2	6	1	2	14.5	-14.2
4	12	1	13.6	-14.3	-1	1	1	18.1	18.7	7	1	2	20.8	-20.9
3	11	1	13.9	-14.4	-3	1	1	28.4	26.6	-5	1	2	35.7	-33.2
-3	11	1	9.3	9.6	-5	1	1	8.2	5.7	5	1	2	47.9	49.5

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-1	3	2	100.1	101.3	-4	6	1	64.9	-64.0	1	9	4	18.0	16.8
1	3	2	57.2	57.0	-2	6	1	66.7	-62.7	9	9	4	8.5	9.5
3	3	2	36.3	36.8	0	6	1	37.1	-36.4	9	9	4	9.8	-10.2
5	3	2	8.0	8.3	2	6	1	30.0	-32.5	9	9	4	21.4	-22.3
8	2	2	6.3	-7.2	4	6	1	11.5	11.5	9	9	4	7.6	8.5
4	2	2	9.0	9.9	6	6	1	15.4	15.0	7	8	4	10.2	-12.1
2	2	2	10.8	12.2	5	5	1	7.3	8.0	8	8	4	11.8	-12.8
0	2	2	88.8	89.5	-1	5	1	12.9	-12.9	8	8	4	15.1	14.0
-2	2	2	42.0	42.1	-3	5	1	43.2	-44.5	8	8	4	12.5	11.7
-4	2	2	22.1	-22.6	-5	5	1	53.7	-54.8	-7	7	4	8.5	-8.2
-6	2	2	10.0	-10.8	-4	4	1	12.5	-12.7	-6	7	4	24.7	-23.5
-7	1	2	8.7	8.3	-2	4	1	25.3	25.2	-3	7	4	13.0	-13.0
-3	1	2	18.3	-18.5	-4	4	1	46.2	47.3	7	7	4	6.7	7.8
-1	1	2	66.1	-69.7	0	4	1	6.5	-6.4	6	6	4	40.1	39.7
1	1	2	88.4	-90.1	2	4	1	5.9	-6.2	6	6	4	94.0	93.5
3	1	2	33.5	-34.4	4	4	1	12.2	-13.0	6	6	4	68.5	65.0
8	0	2	28.9	29.1	7	3	1	26.0	-25.7	6	6	4	26.4	24.0
6	0	2	29.5	30.2	5	3	1	69.2	-69.3	6	6	4	17.7	18.2
4	0	2	24.9	23.8	3	3	1	67.9	-65.1	5	5	4	12.3	-12.4
2	0	2	88.4	89.7	1	3	1	79.1	-76.7	5	5	4	19.3	-19.5
0	0	2	31.1	-36.1	-1	3	1	92.5	-91.6	5	5	4	26.7	-27.4
-2	0	2	46.9	-43.9	-7	3	1	32.8	-32.0	5	5	4	11.0	-11.0
-4	0	2	93.9	92.9	-8	2	1	9.1	-8.1	5	5	4	23.4	24.7
-6	0	2	73.2	72.5	-4	2	1	18.0	18.2	5	5	4	8.6	-9.1
-8	0	2	20.0	20.9	-2	2	1	24.8	26.2	4	4	4	21.8	-22.6
-5	1	2	9.6	9.7	0	2	1	60.2	59.5	4	4	4	24.5	-25.3
-1	1	3	8.8	-9.8	2	2	1	26.5	-26.1	-7	4	4	23.5	24.1
-3	1	3	10.8	-12.0	4	2	1	22.5	-24.1	-1	4	4	20.5	20.8
-4	1	3	25.6	-26.9	1	1	1	37.4	-36.0	-1	4	4	17.8	16.9
-2	1	3	22.7	-23.1	-1	1	1	84.1	-83.0	-7	3	4	34.7	34.4
0	1	3	13.8	-14.9	-3	1	1	67.3	-67.0	-4	3	4	37.4	35.3
-1	1	1	16.4	-17.3	-5	1	1	19.5	-18.9	-1	3	4	37.1	37.6
-3	1	1	11.9	-12.7	-8	0	1	18.1	15.4	-3	4	4	41.8	44.8
-4	1	0	10.9	10.9	-0	0	1	30.8	-30.0	3	4	4	51.6	-47.9
-2	1	0	17.3	16.9	-4	0	1	86.4	-84.1	1	3	4	40.7	-40.0
0	1	0	6.9	6.6	-2	0	1	57.6	-58.4	3	4	4	18.3	18.7
5	9	3	36.1	-35.8	8	0	1	120.6	-116.0	3	4	4	30.3	29.2
3	9	3	39.9	-39.2	2	0	1	40.7	-42.8	2	4	4	9.0	-9.2
1	9	3	22.7	-21.9	4	0	1	24.2	22.6	2	4	4	5.6	-5.2
-1	9	3	16.8	-18.0	8	0	1	13.0	13.6	2	4	4	17.2	-18.3
-4	8	3	14.8	14.7	8	0	1	8.0	-8.3	2	4	4	34.0	36.0
-2	8	3	25.0	24.1	4	1	2	16.3	17.4	-1	4	4	23.0	22.5
0	8	3	9.9	9.4	2	1	2	34.7	35.8	-1	4	4	14.7	-14.1
4	8	3	9.9	-10.9	8	1	2	20.8	22.5	-1	4	4	20.2	-20.7
3	7	3	11.1	11.7	-2	1	2	8.6	8.8	-1	4	4	31.9	-33.7
1	7	3	19.9	-21.2	-5	1	1	12.1	-11.7	-1	4	4	13.6	-11.5
-1	7	3	42.4	-43.2	8	1	0	8.0	-8.7	1	4	4	18.3	15.5
-3	7	3	25.6	-25.0	-4	1	0	10.9	11.2	1	4	4	9.8	-9.9
-5	7	3	13.3	-13.7	-6	1	0	8.5	8.6	1	4	4	10.5	-11.2
-6	6	3	17.8	-16.8	-5	9	4	24.7	24.6	8	6	4	8.5	-8.2

Sample 12. Tas22-1b (continued)

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	5	11	11.9	-12.7	0	4	12	15.3	14.4	-5	1	13	10.5	-11.9
-1	5	11	16.9	-18.0	-2	4	12	15.2	15.5	-6	0	13	26.8	-27.4
-2	4	11	15.6	16.7	-4	4	12	11.9	12.7	-4	0	13	27.7	-27.7
0	4	11	23.2	23.5	-5	1	12	13.4	13.6	0	0	13	24.9	23.9
2	4	11	9.7	9.9	-3	1	12	40.7	42.3	4	0	13	8.8	-8.9
5	3	11	19.1	-20.5	-1	3	12	40.4	40.4	0	6	14	9.2	9.5
3	3	11	7.5	-8.7	3	3	12	16.3	-15.6	-2	6	14	27.6	26.7
-1	3	11	19.7	19.2	-2	2	12	23.5	24.6	-4	6	14	26.3	25.6
-3	3	11	7.1	8.2	-4	2	12	15.7	16.7	-2	4	14	8.7	-10.0
-5	3	11	32.4	-32.5	-3	1	12	12.5	-14.4	-3	3	14	17.6	-17.7
-7	3	11	29.2	-29.4	-1	1	12	12.7	-12.9	1	3	14	8.4	8.9
-6	2	11	17.6	-18.6	3	1	12	8.1	8.7	3	3	14	10.1	9.4
-4	2	11	8.1	-8.1	4	0	12	22.5	23.1	-2	2	14	10.8	-9.0
-2	2	11	7.6	7.9	2	0	12	41.8	40.7	-4	2	14	7.7	-8.2
0	2	11	13.9	14.9	0	0	12	23.6	22.3	3	1	14	8.9	-8.5
2	2	11	18.1	18.2	-2	0	12	20.8	-21.0	2	0	14	6.8	5.5
2	2	11	20.6	19.9	-6	0	12	22.9	23.1	0	0	14	9.0	9.5
1	1	11	16.6	-16.4	-1	0	13	23.9	-23.2	-2	0	14	34.5	33.6
-1	1	11	17.7	-16.8	-4	0	13	24.7	-25.1	-4	0	14	37.8	38.2
-2	0	11	12.9	-13.1	0	0	13	17.4	18.2	-2	6	15	13.4	-10.7
0	0	11	44.6	-45.0	-5	0	13	10.6	-11.2	0	6	15	10.1	-9.6
2	0	11	39.8	-38.6	-4	4	13	11.3	12.3	-3	3	15	10.5	-10.4
-3	9	12	28.4	28.6	3	1	13	9.2	-9.2	0	2	15	11.5	11.3
-1	9	12	24.4	22.9	1	3	13	31.8	-30.8	1	1	15	11.0	-9.7
-2	8	12	11.4	11.7	-1	3	13	46.2	-44.3	-1	1	15	9.8	-9.4
-4	8	12	7.7	8.4	-3	3	13	10.0	-9.8	-2	0	15	9.6	-9.7
-3	7	12	12.2	-13.2	-5	3	13	14.5	15.4	0	0	15	17.9	-17.2
-1	7	12	7.5	-7.6	-6	2	13	9.4	9.5	2	0	15	13.6	-14.0
2	6	12	32.0	32.1	-4	2	13	7.7	8.9	-2	4	16	9.8	9.7
0	6	12	16.1	8.8	2	2	13	7.9	7.5	-3	3	16	10.9	10.9
-2	6	12	12.5	-12.3	1	2	13	7.4	-6.9	-1	3	16	16.7	15.5
-5	5	12	7.9	-8.0	1	1	13	8.6	8.3	-3	1	16	9.0	-9.2
-1	5	12	11.3	-11.4	-3	1	13	7.0	-7.1	-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/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	12	0	64.1	66.0	4	10	1	15.4	16.2	-2	0	1	59.6	57.9
1	11	0	14.7	14.8	3	9	1	7.4	8.4	0	0	1	54.5	-55.6
6	10	0	9.2	10.4	1	9	1	6.8	-8.9	2	0	1	103.2	-103.9
4	10	0	7.2	8.9	-1	9	1	54.5	-54.3	4	0	1	64.1	-64.9
0	10	0	9.1	-8.7	-3	9	1	78.8	-77.0	8	0	1	16.7	-16.9
5	9	0	33.4	34.3	-2	8	1	11.9	-12.7	6	0	1	6.3	-5.8
3	9	0	33.1	34.0	0	8	1	10.8	10.7	-5	1	1	7.1	6.4
1	9	0	34.4	-33.3	2	8	1	29.0	28.2	0	14	2	9.8	10.1
6	8	0	13.3	13.4	4	8	1	20.8	20.0	-1	13	2	9.7	-9.8
4	8	0	12.7	13.1	6	8	1	7.6	7.1	1	13	2	15.4	-16.5
0	8	0	8.1	-8.1	5	7	1	17.7	-16.3	4	12	2	8.5	9.9
7	7	0	7.4	-8.0	3	7	1	33.6	-32.2	-1	11	2	22.0	-23.5
5	7	0	11.1	-10.7	-3	7	1	13.6	13.1	1	11	2	19.4	-19.9
3	7	0	7.3	-7.5	-5	7	1	9.6	9.7	3	11	2	8.0	-8.1
1	7	0	30.6	30.8	-4	6	1	33.4	30.8	2	10	2	16.9	17.3
4	6	0	7.0	5.8	-2	6	1	62.2	62.1	0	10	2	23.2	23.3
2	6	0	98.9	98.2	0	6	1	54.9	-53.1	-2	10	2	8.8	9.3
0	6	0	171.3	170.6	2	6	1	88.3	-87.7	-3	9	2	18.4	20.5
7	5	0	11.7	-11.1	4	6	1	36.0	-35.0	-1	9	2	72.9	70.8
5	5	0	18.5	-17.4	6	6	1	17.3	-16.4	1	9	2	40.6	38.6
3	5	0	11.2	11.4	5	5	1	15.1	-14.8	3	9	2	18.4	18.6
1	5	0	19.7	20.7	3	5	1	31.6	-30.3	5	9	2	11.0	11.3
8	4	0	6.5	6.4	1	5	1	41.6	-42.8	2	8	2	24.8	24.1
6	4	0	24.1	22.4	-1	5	1	21.7	21.7	0	8	2	30.5	30.2
4	4	0	19.5	19.0	-3	5	1	27.8	27.0	-2	8	2	12.6	12.7
0	4	0	32.5	31.1	0	4	1	30.8	-31.0	-6	8	2	9.1	-9.2
7	3	0	24.2	23.0	-2	4	1	38.5	37.7	-1	7	2	50.2	-49.2
5	3	0	64.8	62.1	2	4	1	58.3	56.8	1	7	2	38.0	-37.1
3	3	0	52.5	50.8	4	4	1	26.9	25.7	3	7	2	14.6	-13.7
1	3	0	59.3	-58.3	6	4	1	11.4	11.0	6	6	2	25.2	23.9
8	2	0	8.9	8.4	7	3	1	9.9	-10.0	4	6	2	26.9	25.0
6	2	0	16.7	16.9	5	3	1	18.4	-17.4	2	6	2	19.3	18.7
4	2	0	33.3	32.4	1	3	1	43.7	41.7	-4	6	2	52.6	50.7
2	2	0	35.5	34.7	-1	3	1	132.9	-130.2	-6	6	2	58.1	55.4
0	2	0	45.7	-45.1	-3	3	1	164.8	-163.1	-3	5	2	15.3	-15.6
7	1	0	12.1	-12.3	-5	3	1	59.6	-48.0	-1	5	2	32.0	-31.5
5	1	0	18.8	-19.0	-4	2	1	17.9	-18.8	1	5	2	66.6	-65.4
3	1	0	6.6	6.7	-2	2	1	29.4	25.1	3	5	2	30.7	-29.3
1	1	0	41.0	40.0	0	2	1	8.9	9.8	6	4	2	8.8	-0.7
2	0	0	128.9	127.8	2	2	1	40.9	42.1	2	4	2	54.1	54.0
0	0	0	7.0	5.9	4	2	1	49.0	50.8	8	4	2	37.9	39.2
1	1	1	8.7	-10.2	8	2	1	8.1	8.1	-3	4	2	13.5	14.2
1	1	1	7.5	8.7	5	1	1	19.4	-20.4	-6	4	2	13.9	-12.8
2	1	1	37.0	-38.3	3	1	1	44.5	-44.1	-5	3	2	30.6	-29.8
4	1	1	17.0	-18.4	1	1	1	43.0	-43.3	-3	3	2	53.3	51.1
5	1	1	8.0	-8.5	-1	1	1	18.8	17.1	-1	3	2	108.1	105.6
3	1	1	16.0	-16.9	-3	1	1	28.1	28.1	1	3	2	61.3	60.5
-3	1	1	9.0	10.0	-8	0	1	25.6	-23.8	3	3	2	38.3	38.2
-2	1	1	9.5	-9.5	-6	0	1	18.0	-17.8	5	3	2	9.8	8.9
2	1	1	19.1	19.9	-4	0	1	60.3	58.1	7	3	2	7.5	-7.2

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
4	2	2	9.9	9.3	-3	7	3	27.5	-26.8	-2	12	4	11.7	12.7
2	2	2	10.5	10.7	-5	7	3	14.0	-13.4	-5	11	4	11.9	-13.4
0	2	2	87.1	88.0	-6	6	3	18.9	-17.2	-3	11	4	8.8	-8.2
-2	2	2	41.1	42.9	-4	6	3	67.1	-65.8	2	10	4	10.1	-10.1
-4	2	2	22.4	-22.0	-2	6	3	71.0	-70.2	0	10	4	9.0	-9.7
-6	2	2	9.9	-9.1	0	6	3	40.6	-40.4	-4	10	4	11.9	12.7
-5	1	2	9.7	9.8	2	6	3	35.5	-34.4	-6	10	4	8.6	8.8
-3	1	2	17.7	-17.6	4	6	3	10.7	9.7	-5	9	4	27.6	26.5
-1	1	2	64.8	-67.8	6	6	3	12.9	13.0	-3	9	4	20.9	20.1
1	1	2	86.1	-88.6	5	5	3	7.2	7.1	-1	9	4	10.6	10.9
3	1	2	34.7	-34.8	1	5	3	14.8	-14.0	1	9	4	10.7	-9.9
8	0	2	23.7	25.5	-1	5	3	47.1	-47.1	3	9	4	21.7	-22.2
6	0	2	27.6	28.9	-3	5	3	56.5	-55.1	5	9	4	9.7	10.0
4	0	2	24.4	24.7	-5	5	3	13.2	-11.7	2	8	4	13.1	-12.8
2	0	2	92.6	92.2	4	4	3	25.8	24.8	0	8	4	14.5	-14.5
0	0	2	23.3	-22.1	-2	4	3	49.7	49.4	-2	8	4	5.8	5.7
-2	0	2	40.0	-40.6	0	4	3	6.7	-7.0	-4	8	4	15.0	14.6
-4	0	2	92.6	92.5	4	4	3	13.4	-13.8	-6	8	4	12.7	11.3
-6	0	2	68.2	67.3	6	4	3	8.5	-8.1	-7	7	4	7.9	-7.2
-7	1	2	7.1	7.0	7	3	3	23.5	-24.8	-5	7	4	24.2	-23.6
-7	3	2	19.8	-17.1	5	3	3	68.7	-68.1	-3	7	4	14.5	-14.5
-7	5	2	7.5	7.4	3	3	3	70.2	-69.8	-1	7	4	7.5	8.1
-5	5	2	6.9	6.9	1	3	3	80.9	-81.4	3	7	4	7.8	7.2
-5	7	2	10.1	10.2	-1	3	3	93.5	-94.7	4	6	4	43.0	41.9
-2	14	3	8.6	10.9	-5	3	3	6.6	-5.1	2	6	4	101.8	99.8
-1	13	3	10.8	-12.6	-7	3	3	31.9	-29.1	0	6	4	74.2	73.2
-3	13	3	12.2	-14.0	-8	2	3	6.5	-6.7	-2	6	4	27.7	26.7
-4	12	3	29.1	-31.2	-4	2	3	17.8	18.3	-4	6	4	19.8	19.0
-2	12	3	27.3	-29.0	-2	2	3	24.4	24.7	-7	5	4	11.3	-11.0
0	12	3	18.5	-19.8	0	2	3	58.7	60.1	-5	5	4	19.8	-19.6
1	11	3	7.4	-7.8	2	2	3	25.1	-27.0	-3	5	4	29.0	-27.6
-1	11	3	20.4	-20.9	4	2	3	23.1	-23.8	-1	5	4	11.3	-11.2
-3	11	3	14.1	-14.5	5	1	3	6.3	6.3	1	5	4	24.4	25.4
-4	10	3	10.8	11.3	1	1	3	37.6	-38.0	5	5	4	9.2	-8.9
-2	10	3	19.3	19.6	-1	1	3	81.8	-81.7	4	4	4	6.8	5.9
0	10	3	8.0	9.0	-3	1	3	65.2	-66.1	2	4	4	23.4	-23.2
2	10	3	7.6	-8.9	5	1	3	17.1	-17.0	0	4	4	25.4	-26.6
4	10	3	8.5	-8.5	-8	0	3	12.5	11.7	-2	4	4	24.3	24.4
5	9	3	37.9	-38.4	-6	0	3	30.6	-29.1	-4	4	4	20.2	19.7
3	9	3	46.4	-45.0	-4	0	3	82.1	-84.1	-6	4	4	16.3	15.4
1	9	3	28.6	-27.0	-2	0	3	60.1	-60.1	-7	3	4	32.9	31.0
-1	9	3	20.7	-20.6	0	0	3	117.2	-118.7	-5	3	4	36.4	35.3
-3	9	3	6.2	-6.4	2	0	3	41.5	-43.8	-3	3	4	38.3	39.3
-4	8	3	15.2	15.2	4	0	3	19.0	19.4	-1	3	4	45.0	45.6
-2	8	3	27.8	27.4	6	0	3	10.3	10.4	1	3	4	46.8	-46.9
0	8	3	10.3	10.2	2	4	3	5.9	-6.0	3	3	4	38.5	-37.8
4	8	3	11.5	-11.3	1	13	4	7.8	8.7	5	3	4	18.6	18.0
3	7	3	12.1	12.1	4	12	4	20.2	21.5	7	3	4	26.5	27.5
1	7	3	22.8	-22.1	2	12	4	41.1	43.4	8	2	4	9.6	10.7
-1	7	3	47.7	-46.2	0	12	4	28.2	29.2	4	2	4	9.2	-8.7

