

Observed and calculated structure factors for biotite-1M crystals: GFS15a

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	1	1	37.1	-37.3	1	9	0	11.1	-11.1	1	1	11	12.8	-13.0
1	1	0	28.5	27.6	-1	9	1	55.3	-57.5	1	1	10	13.8	-13.6
-1	1	1	12.5	12.0	-1	9	2	71.9	71.9	1	1	7	24.4	-25.5
-1	1	2	63.6	-63.4	-1	9	3	31.6	-33.8	1	1	6	26.8	-28.3
-1	1	3	83.8	-83.3	-1	9	4	18.2	20.5	1	1	4	9.0	8.2
-1	1	4	16.8	-16.4	-1	9	5	76.0	-79.2	1	1	3	43.3	-41.9
-1	1	5	10.0	9.2	-1	9	6	27.6	31.1	1	1	2	88.1	-87.1
-1	1	6	5.4	-7.0	-1	9	7	9.7	8.9	0	12	5	5.5	4.8
-1	1	7	36.2	-36.2	-1	9	8	13.1	14.4	0	12	4	31.9	31.5
-1	1	8	14.8	-15.1	-1	9	9	36.9	-38.3	0	12	3	28.9	-29.2
-1	1	9	4.7	4.9	1	11	0	16.0	16.0	0	12	2	7.6	6.4
-1	1	10	5.9	-5.3	-1	11	2	22.6	-21.4	0	12	1	25.0	-23.7
-1	1	11	15.1	-15.7	-1	11	3	21.0	-19.7	0	12	0	65.9	64.7
-1	1	12	10.0	-10.0	-1	11	4	3.8	3.1	0	10	9	6.3	-7.5
-1	1	13	5.0	4.6	-1	11	5	13.7	13.4	0	10	7	11.5	12.7
-1	1	14	4.7	4.6	-1	11	7	15.2	-15.4	0	10	6	13.0	12.9
1	3	0	26.1	-24.9	1	11	6	6.5	-7.3	0	10	4	6.1	-6.3
-1	3	4	63.4	65.4	1	11	3	10.9	-10.5	0	10	3	7.4	8.1
-1	3	6	62.3	63.6	1	11	2	16.1	-15.1	0	10	2	20.6	20.2
-1	3	7	7.8	7.5	1	9	9	31.7	-32.4	0	10	0	4.2	-5.6
-1	3	8	4.8	3.5	1	9	7	26.8	-28.6	0	8	11	11.8	13.8
-1	3	9	72.8	-72.0	1	9	6	60.1	60.7	0	8	9	10.4	-13.5
-1	3	10	6.9	7.5	1	9	5	48.0	-48.5	0	8	8	5.5	-6.4
-1	3	11	8.6	-7.9	1	9	4	6.8	5.2	0	8	7	21.1	22.7
-1	3	12	47.5	47.9	1	9	3	36.5	-37.6	0	8	6	25.0	27.4
-1	3	13	47.9	-47.0	1	9	2	40.5	42.1	0	8	4	11.9	-12.0
1	5	1	36.6	-38.4	1	7	11	8.9	-9.2	0	8	2	22.0	22.4
1	5	0	19.9	18.3	1	7	10	12.3	-12.8	0	8	1	13.2	14.0
-1	5	1	14.3	16.3	1	7	8	5.3	5.4	0	6	12	14.2	14.6
-1	5	2	32.0	-31.3	1	7	7	7.0	-8.1	0	6	11	42.9	-44.7
-1	5	3	45.2	-45.3	1	7	6	9.7	-11.2	0	6	10	36.8	39.8
-1	5	4	13.6	-13.7	1	7	3	23.0	-23.0	0	6	9	7.0	-8.0
-1	5	5	4.8	4.0	1	7	2	34.3	-32.6	0	6	8	62.0	63.2
-1	5	7	24.9	-25.2	1	5	11	9.6	-10.2	0	6	7	60.8	-62.7
-1	5	8	5.5	-4.9	1	5	10	6.8	-7.5	0	6	6	8.7	8.3
-1	5	9	6.0	6.3	1	5	7	21.4	-23.4	0	6	5	17.5	17.7

-1	5	10	6.0	-5.8	1	5	6	26.4	-27.3	0	6	4	80.8	80.0
-1	5	11	14.6	-15.2	1	5	5	6.2	5.9	0	6	3	47.0	-47.2
-1	5	12	9.0	-9.1	1	5	4	17.8	18.9	0	6	2	30.1	31.7
-1	5	13	6.7	6.2	1	5	3	20.4	-19.6	0	6	1	70.8	-69.1
1	7	0	26.6	25.7	1	3	13	34.6	-33.8	0	6	0	164.6	165.7
-1	7	2	39.7	-41.8	1	3	12	8.7	8.3	0	4	13	4.2	-4.1
-1	7	3	41.8	-43.7	1	3	11	8.9	8.6	0	4	12	15.6	15.3
-1	7	4	5.9	4.8	1	3	10	20.0	19.8	0	4	11	20.5	21.8
-1	7	5	20.2	20.0	1	3	9	63.4	-63.9	0	4	10	4.0	4.0
-1	7	7	24.8	-26.8	1	3	7	43.8	-44.3	0	4	9	21.9	-24.2
-1	7	8	14.4	-15.2	1	3	4	14.3	-14.0	0	4	8	9.8	-10.1
-1	7	11	5.5	-5.8	1	3	3	96.1	-98.2	0	4	7	36.6	39.1
-1	7	12	4.4	-4.7	1	3	2	61.6	62.3	0	4	6	52.7	53.9
1	9	1	22.6	-21.7	1	1	13	6.8	7.0	0	4	5	15.3	15.4

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0	4	4	22.3	-22.8	2	8	5	7.6	6.9	-2	0	4	102.6	101.4
0	4	3	14.8	-13.7	2	8	4	12.2	-12.5	-2	0	5	16.9	16.7
0	4	2	27.7	29.9	2	8	2	21.0	23.4	-2	0	6	118.2	117.9
0	4	1	40.0	40.3	2	8	1	25.9	25.9	-2	0	7	136.8	-135.3
0	4	0	49.0	49.8	-2	8	1	15.3	-14.3	-2	0	8	44.3	44.6
0	2	13	8.0	-7.9	2	6	11	25.6	-27.3	-2	0	10	70.5	68.8
0	2	12	6.2	5.1	2	6	10	9.6	11.1	-2	0	11	21.8	-20.5
0	2	11	15.8	15.5	2	6	9	11.6	-12.6	-2	0	12	10.2	-9.6
0	2	10	11.2	10.7	2	6	8	37.7	37.9	-2	0	13	10.5	-9.6
0	2	7	32.1	31.9	2	6	7	14.9	-14.2	-2	0	14	36.3	36.1
0	2	6	19.0	20.9	2	6	6	7.7	4.8	-2	2	2	42.8	43.5
0	2	5	11.1	-9.9	2	6	5	24.1	-23.2	-2	2	3	13.4	16.1
0	2	4	6.0	5.0	2	6	4	107.5	105.4	-2	2	4	25.7	-23.0
0	2	1	8.5	8.4	2	6	3	54.8	-53.0	-2	2	5	15.9	-14.9
0	2	0	31.2	-31.7	2	6	2	33.1	31.2	-2	2	6	33.6	32.0
0	0	14	12.7	12.4	2	6	1	96.9	-94.7	-2	2	7	58.5	57.9
0	0	13	13.5	13.4	2	6	0	113.3	111.9	-2	2	8	25.8	25.6
0	0	12	31.8	30.5	-2	6	1	44.4	43.7	-2	2	9	25.7	-24.2
0	0	11	49.6	-49.3	2	4	11	7.2	7.8	-2	2	10	17.1	-16.2
0	0	10	49.8	48.7	2	4	10	9.4	9.9	-2	2	11	13.1	11.7
0	0	9	33.6	-33.7	2	4	8	6.4	-5.4	-2	2	12	25.9	24.6
0	0	7	69.7	-70.4	2	4	7	14.5	15.2	-2	2	13	9.5	8.6

0	0	6	54.3	55.6	2	4	6	29.3	30.9	-2	2	14	7.8	-7.6
0	0	2	19.4	18.0	2	4	5	6.4	6.6	-2	4	2	10.7	12.9
0	0	1	75.6	-76.2	2	4	4	19.8	-18.5	-2	4	3	49.8	47.6
0	0	4	78.3	75.4	2	4	2	53.9	53.2	-2	4	4	30.4	28.0
0	0	5	77.2	75.8	2	4	1	52.0	50.6	-2	4	6	3.6	3.8
0	0	8	78.0	75.1	-2	4	1	25.1	-26.3	-2	4	7	21.2	18.8
-1	3	1	142.4	-140.7	2	2	11	19.4	20.2	-2	4	8	16.4	15.5
1	3	5	115.0	-113.6	2	2	10	17.0	18.0	-2	4	9	9.5	-7.1
1	3	6	129.9	128.8	2	2	9	7.3	-6.7	-2	4	11	15.9	14.3
1	7	1	5.5	-4.0	2	2	8	23.9	-25.2	-2	4	12	14.5	12.8
-1	5	6	8.4	-8.0	2	2	7	5.4	5.1	-2	6	2	24.0	22.5
-1	3	5	145.3	-142.9	2	2	6	51.2	51.4	-2	6	3	83.4	-81.8
-1	3	3	127.4	-124.8	2	2	5	47.1	44.6	-2	6	4	36.2	34.3
-1	3	2	120.5	117.6	2	2	3	27.3	-26.6	-2	6	6	94.2	92.3
2	12	3	17.5	-19.1	2	2	1	34.0	35.5	-2	6	7	72.5	-72.1
2	12	2	14.8	15.8	2	2	0	44.5	47.6	-2	6	8	36.2	35.0
2	12	1	37.3	-38.5	-2	2	1	41.6	43.1	-2	6	9	14.2	-13.4
2	12	0	39.0	39.3	2	0	12	44.5	44.6	-2	6	10	39.3	37.5
2	10	6	17.1	18.0	2	0	11	42.7	-45.0	-2	6	11	22.1	-20.2
2	10	5	8.3	9.5	2	0	10	7.1	8.1	-2	8	2	12.4	12.2
2	10	4	5.9	-6.3	2	0	9	7.8	-7.6	-2	8	3	24.1	23.7
2	10	3	8.2	-9.3	2	0	8	68.3	69.2	-2	8	4	9.4	9.1
2	10	2	11.5	11.1	2	0	6	8.9	-6.6	-2	8	5	6.8	-6.5
2	10	1	14.3	14.3	2	0	5	61.3	-61.8	-2	8	7	18.3	17.2
2	10	0	5.3	4.7	2	0	3	62.6	-64.3	-2	8	8	10.3	9.7
2	8	8	5.9	-6.5	2	0	1	113.9	-116.9	-2	8	9	9.1	-7.8
2	8	7	5.6	6.3	-2	0	1	24.1	24.4	-2	8	11	8.7	8.2
2	8	6	20.7	21.4	-2	0	3	62.3	-64.5	-2	10	2	8.8	8.8
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-2	10	3	11.7	11.5	3	9	2	24.5	25.3	-3	1	10	6.6	7.2
-2	10	5	6.5	-7.9	3	9	3	52.4	-53.2	-3	1	9	7.0	-6.7
-2	10	6	6.6	6.7	3	9	4	10.5	-8.4	-3	1	8	32.8	-32.7
-2	10	7	13.1	15.3	3	9	6	42.7	42.9	-3	1	7	19.3	-19.3
-2	10	8	8.1	9.0	3	9	7	32.3	-32.7	-3	1	6	15.8	16.4
-2	12	3	36.4	-33.9	-3	11	1	8.2	9.2	-3	1	5	11.4	11.3
-2	12	4	20.4	20.3	3	11	1	14.1	-15.4	-3	1	4	33.5	-35.0

Observed and calculated structure factors for biotite-1M crystals: GFS15a

-3	1	1	21.2	22.7	3	11	2	7.6	-7.4	-3	1	3	63.5	-66.3
3	1	1	40.8	-41.9	3	11	3	5.7	5.8	-3	1	2	13.2	-15.9
3	1	2	37.0	-38.4	-3	11	4	6.4	-6.4	4	10	3	8.9	-9.5
3	1	3	4.8	-4.8	-3	11	3	13.6	-13.5	4	10	1	14.4	15.2
3	1	5	15.8	-16.3	-3	9	9	45.0	-43.7	4	10	0	9.9	9.9
3	1	6	19.6	-18.9	-3	9	8	36.5	34.6	-4	10	1	6.4	-6.3
3	1	8	4.0	3.3	-3	9	5	41.2	-40.6	4	8	6	9.6	9.7
3	1	9	9.7	-10.6	-3	9	4	28.0	27.7	4	8	5	20.1	19.3
3	1	10	12.7	-14.7	-3	9	3	22.7	-22.1	4	8	3	11.9	-11.5
-3	3	1	168.0	-169.7	-3	9	2	27.2	28.2	4	8	1	14.8	14.7
3	3	0	70.1	70.3	-3	7	11	8.8	-6.8	4	8	0	14.4	14.2
3	3	1	32.8	-30.9	-3	7	10	8.8	7.9	4	6	8	29.6	31.8
3	3	2	48.9	47.2	-3	7	8	16.0	-15.0	4	6	6	29.4	29.2
3	3	3	84.0	-82.0	-3	7	7	16.7	-14.4	4	6	5	62.5	-60.2
3	3	4	19.3	-17.6	-3	7	6	3.8	3.3	4	6	4	49.7	48.5
3	3	5	10.5	-8.1	-3	7	5	4.0	3.6	4	6	3	7.6	-5.5
3	3	6	64.1	62.2	-3	7	4	14.9	-14.5	4	6	2	40.5	38.4
3	3	7	63.1	-62.3	-3	7	3	25.4	-26.0	4	6	1	42.1	-43.4
3	3	8	6.6	7.2	-3	5	12	6.5	-6.4	4	6	0	24.4	23.8
3	3	9	38.3	-38.7	-3	5	10	4.4	5.2	-4	6	1	14.4	12.1
3	3	10	43.0	43.2	-3	5	9	8.5	-7.6	4	4	9	7.4	7.7
3	3	11	14.3	-14.1	-3	5	8	31.0	-28.7	4	4	8	9.8	-10.0
-3	5	1	24.5	25.0	-3	5	7	14.9	-13.9	4	4	7	11.5	-11.2
3	5	0	11.5	9.6	-3	5	6	22.5	20.4	4	4	6	15.2	14.0
3	5	1	29.1	-27.8	-3	5	5	14.8	13.8	4	4	5	29.4	29.2
3	5	2	32.8	-30.4	-3	5	4	27.2	-27.0	4	4	4	12.2	11.7
3	5	3	7.9	-6.9	-3	5	3	53.8	-54.9	4	4	3	13.5	-13.0
3	5	5	12.0	-10.7	-3	5	2	13.9	-14.8	4	4	2	4.9	-4.8
3	5	6	11.3	-11.4	-3	3	13	18.7	-16.1	4	4	1	18.9	18.6
3	5	9	11.0	-10.0	-3	3	12	49.8	48.6	4	4	0	19.6	19.8
3	5	10	13.4	-12.9	-3	3	11	43.2	-42.1	-4	4	1	4.9	5.4
-3	7	1	10.8	10.3	-3	3	10	9.2	8.0	4	2	10	6.1	6.2
3	7	0	7.5	-6.4	-3	3	9	67.8	-66.9	4	2	6	21.2	21.9
3	7	1	31.0	-29.7	-3	3	8	66.5	66.2	4	2	5	22.3	22.6
3	7	2	16.9	-14.9	-3	3	7	11.0	-9.3	4	2	4	9.3	-9.0
3	7	3	10.7	9.1	-3	3	6	19.2	-18.7	4	2	3	22.3	-22.9
3	7	4	7.8	6.3	-3	3	5	84.9	-83.7	4	2	2	13.8	13.0
3	7	5	14.9	-13.7	-3	3	4	50.5	50.4	4	2	1	48.8	51.2
3	7	6	18.1	-17.1	-3	3	3	31.1	-32.9	4	2	0	32.5	34.1

3	7	8	6.2	6.3	-3	3	2	67.2	69.0	-4	2	1	13.3	-15.7
-3	9	1	77.1	-76.2	-3	1	13	5.9	-6.3	4	0	9	18.9	-19.5
3	9	0	44.9	44.2	-3	1	12	10.1	-10.6	4	0	8	33.3	35.1
3	9	1	7.1	-6.8	-3	1	11	5.3	-5.7	4	0	7	12.7	-11.8
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
4	0	6	32.9	34.3	-4	8	4	10.7	9.6	-5	5	10	9.4	9.4
4	0	5	67.3	-69.3	-4	8	5	5.2	-6.1	-5	5	9	11.1	-11.8
4	0	4	86.6	89.2	-4	8	6	5.2	-4.3	-5	5	8	16.8	-18.5
4	0	2	35.6	35.6	-4	8	7	9.7	10.0	-5	5	6	10.0	9.9
4	0	1	80.0	-82.5	-4	8	8	19.5	19.6	-5	5	2	7.5	8.0
4	0	0	23.0	23.4	-4	10	2	6.0	-5.3	-5	3	11	37.8	-38.7
-4	0	1	43.8	45.0	-4	10	3	6.9	7.5	-5	3	9	30.4	-31.7
-4	0	2	115.7	116.8	-4	10	4	13.8	13.1	-5	3	8	66.8	68.1
-4	0	3	97.3	-98.5	-5	1	1	5.4	5.5	-5	3	7	53.1	-54.2
-4	0	4	30.0	31.3	5	1	0	16.6	-17.9	-5	3	6	5.6	4.6
-4	0	5	53.1	-56.0	5	1	1	22.8	-23.1	-5	3	5	38.8	-40.5
-4	0	6	113.7	114.5	5	1	3	6.1	5.9	-5	3	3	24.8	-25.5
-4	0	7	24.1	-25.3	5	1	4	9.7	-9.9	-5	3	2	12.4	-13.1
-4	0	8	6.7	5.1	5	1	5	16.2	-16.0	-5	1	10	6.3	7.3
-4	0	9	16.7	-16.4	5	1	6	4.1	-3.4	-5	1	9	17.7	-17.8
-4	0	10	41.3	43.6	5	1	7	7.7	7.9	-5	1	8	19.5	-20.7
-4	0	11	12.7	-13.9	-5	3	1	61.9	-60.9	-5	1	6	12.3	14.5
-4	0	12	9.9	11.4	5	3	0	78.5	76.2	-5	1	5	5.0	-5.4
-4	0	13	31.4	-31.8	5	3	1	35.6	-33.6	-5	1	4	30.0	-32.0
-4	2	2	20.8	-23.4	5	3	2	19.7	18.6	-5	1	3	18.7	-20.0
-4	2	3	16.0	17.7	5	3	3	80.9	-81.3	-5	1	2	9.5	10.4
-4	2	4	35.3	37.4	5	3	4	30.8	31.2	6	6	2	35.7	34.5
-4	2	5	13.7	14.8	5	3	5	11.2	9.0	6	6	1	30.5	-30.7
-4	2	7	3.8	3.6	5	3	6	15.0	14.9	6	4	5	15.4	14.8
-4	2	8	15.5	15.9	5	3	7	39.9	-38.3	6	4	4	7.3	6.6
-4	2	10	5.8	-5.0	5	5	0	18.1	-16.6	6	4	3	11.0	-10.8
-4	2	11	8.3	8.8	5	5	1	15.6	-16.0	6	4	2	10.5	-11.2
-4	2	12	14.1	15.8	5	5	3	8.4	7.7	6	4	1	15.6	14.6
-4	2	13	6.2	6.2	5	5	4	9.9	-9.3	6	4	0	27.8	27.0
-4	4	2	7.6	8.5	5	5	5	17.1	-15.8	-6	4	1	6.6	7.1
-4	4	3	20.7	22.3	5	5	7	8.8	7.9	6	2	5	14.1	13.8
-4	4	4	12.1	13.9	-5	7	1	11.3	10.6	6	2	4	16.2	15.2

-4	4	5	12.8	-13.8	5	7	0	8.3	-7.4	6	2	2	8.0	-8.7
-4	4	6	5.8	-5.1	5	7	1	19.0	-17.7	6	2	1	6.1	6.1
-4	4	7	18.0	18.9	5	7	2	6.4	-4.6	6	2	0	14.4	14.7
-4	4	8	31.7	32.4	5	7	5	6.7	-6.2	-6	2	1	5.5	5.1
-4	4	9	4.5	4.1	-5	9	1	41.2	-41.3	6	0	6	44.7	42.1
-4	4	10	14.6	-16.4	5	9	0	40.0	41.1	6	0	5	35.9	-32.9
-4	4	11	6.0	-5.1	5	9	1	16.6	-15.6	6	0	2	41.6	42.1
-4	4	12	11.0	12.8	5	9	2	19.3	18.5	6	0	1	27.9	-27.9
-4	6	2	61.2	59.7	-5	9	5	22.7	-21.1	6	0	0	22.2	22.6
-4	6	3	76.5	-76.0	-5	9	4	37.9	37.0	-6	0	1	25.9	-28.6
-4	6	4	33.0	34.4	-5	7	9	15.9	-15.3	-6	0	2	81.1	81.5
-4	6	5	20.1	-19.7	-5	7	8	11.0	-10.9	-6	0	3	47.1	-47.3
-4	6	6	85.8	85.6	-5	7	7	6.5	6.0	-6	0	5	28.9	-29.2
-4	6	7	33.1	-33.5	-5	7	6	14.8	14.9	-6	0	6	63.0	63.1
-4	6	8	11.7	-10.8	-5	7	5	5.7	-5.7	-6	0	7	12.2	10.9
-4	6	9	15.1	-16.6	-5	7	4	26.2	-26.3	-6	0	9	53.5	-52.9
-4	6	10	41.0	42.8	-5	7	3	16.3	-15.6	-6	0	10	40.1	38.4
-4	8	3	13.8	13.6	-5	7	2	10.9	10.9	-6	2	3	6.8	7.6

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-6	2	4	21.5	21.4	-6	4	9	6.5	6.1	7	3	1	21.9	-22.4
-6	2	6	11.1	-11.9	-6	6	2	71.8	70.6	-7	3	6	23.4	21.4
-6	2	7	4.6	-4.4	-6	6	4	7.5	6.5	-7	3	5	14.9	-15.6
-6	2	8	18.4	18.0	-6	6	5	34.6	-33.6	-7	3	4	43.9	43.8
-6	2	9	19.9	19.6	-6	6	6	38.1	37.3	-7	3	3	46.9	-46.0
-6	4	2	14.3	-14.5	-6	6	7	7.1	5.5	-7	1	7	8.1	8.5
-6	4	3	8.2	-9.0	-7	1	1	4.3	-4.6	-7	1	6	4.7	5.1
-6	4	4	17.6	16.5	7	1	0	14.3	-13.9	-7	1	5	15.1	-15.3
-6	4	5	14.8	15.4	-7	3	1	9.8	-10.4	-7	1	4	16.6	-15.9
-6	4	6	4.0	2.9	7	3	0	40.4	38.6	-7	1	2	8.0	8.1
-6	4	8	5.7	5.2										