

Observed and calculated structure factors for biotite-1M crystals: H87

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1	1	1	38.6	-37.2	-1	9	2	84.5	86.0	1	5	5	7.6	7.7
1	1	0	31.9	32.0	-1	9	3	36.8	-37.6	1	5	4	22.8	22.1
-1	1	1	15.4	16.1	-1	9	4	20.1	22.2	1	5	3	20.9	-20.3
-1	1	2	63.5	-63.4	-1	9	5	96.8	-95.5	1	5	2	61.0	-61.7
-1	1	3	81.6	-81.5	-1	9	6	35.1	35.5	1	3	15	13.3	-11.9
-1	1	4	16.8	-16.6	-1	9	7	12.4	11.7	1	3	14	15.0	15.0
-1	1	5	10.7	10.6	-1	9	8	17.2	17.8	1	3	13	36.0	-35.9
-1	1	6	5.5	-5.5	-1	9	9	45.5	-46.0	1	3	12	9.5	9.6
-1	1	7	34.2	-35.4	-1	9	12	31.4	34.0	1	3	11	10.0	9.8
-1	1	8	14.8	-15.2	-1	9	13	28.8	-30.3	1	3	10	20.8	20.1
-1	1	9	5.0	5.2	1	11	0	20.2	21.7	1	3	9	68.8	-68.5
-1	1	10	5.5	-5.1	-1	11	2	29.0	-30.1	1	3	7	45.9	-45.7
-1	1	11	15.0	-15.1	-1	11	3	24.5	-26.1	1	3	6	135.6	135.7
-1	1	12	11.1	-10.0	-1	11	5	18.5	18.9	1	3	5	121.4	-118.7
-1	1	15	8.6	-8.5	-1	11	7	21.0	-22.0	1	3	4	15.6	-13.5
-1	1	16	7.0	-7.0	-1	11	8	8.9	-9.4	1	3	2	69.8	68.6
1	3	0	19.0	-19.2	1	13	1	12.0	-12.9	1	1	15	9.3	-9.1
-1	3	4	68.8	69.5	1	13	0	9.3	9.9	1	1	13	7.2	7.1
-1	3	6	66.5	66.8	-1	13	2	7.5	-8.2	1	1	11	14.0	-13.1
-1	3	7	6.7	6.3	-1	13	3	15.1	-16.5	1	1	10	14.0	-13.6
-1	3	9	73.9	-73.9	-1	13	7	9.9	-9.8	1	1	7	26.5	-26.4
-1	3	11	7.5	-7.6	1	13	7	10.6	-11.6	1	1	6	26.2	-27.8
-1	3	12	50.8	49.9	1	13	6	9.4	-9.8	1	1	4	9.9	10.0
-1	3	13	48.4	-48.2	1	13	4	12.3	12.6	1	1	3	43.1	-42.4
-1	3	15	16.1	-13.8	1	13	2	19.2	-20.2	1	1	2	86.5	-86.6
-1	3	16	18.9	18.5	1	11	10	9.0	-9.2	0	14	2	13.2	13.2
1	5	1	40.5	-42.8	1	11	8	5.9	5.5	0	14	1	4.3	4.4
1	5	0	18.6	19.8	1	11	6	10.6	-11.3	0	12	9	8.8	-9.4
-1	5	1	17.2	19.1	1	11	3	15.1	-14.8	0	12	8	33.6	35.0
-1	5	2	31.9	-32.0	1	11	2	18.9	-20.1	0	12	7	37.5	-37.8
-1	5	3	46.2	-46.2	1	9	11	7.5	7.9	0	12	6	10.0	10.2
-1	5	4	15.8	-15.6	1	9	10	23.2	22.7	0	12	5	8.6	8.3
-1	5	6	7.9	-8.3	1	9	9	38.2	-39.9	0	12	4	43.4	44.0
-1	5	7	26.3	-26.5	1	9	7	33.6	-34.2	0	12	3	37.3	-37.8
-1	5	9	6.7	6.7	1	9	6	73.0	72.1	0	12	2	6.8	7.0
-1	5	11	14.9	-16.3	1	9	5	58.1	-58.2	0	12	1	26.8	-29.8

-1 5 12 10.1 -10.2 1 9 3 44.0 -43.9 0 12 0 85.8 86.9
-1 5 13 6.9 6.9 1 9 2 50.2 50.6 0 10 12 5.4 5.7
-1 5 14 6.7 6.1 1 7 13 9.2 8.9 0 10 11 9.8 10.7
-1 5 15 7.2 -7.0 1 7 11 9.9 -10.8 0 10 10 5.1 4.9
1 7 0 26.9 28.7 1 7 10 14.1 -15.2 0 10 9 9.3 -9.6
-1 7 2 47.2 -48.3 1 7 8 5.7 5.8 0 10 7 15.7 16.5
-1 7 3 47.9 -48.6 1 7 7 9.1 -8.9 0 10 6 17.3 17.1
-1 7 5 23.0 23.4 1 7 6 12.8 -12.3 0 10 4 6.9 -7.5
-1 7 7 30.2 -30.7 1 7 3 26.3 -26.8 0 10 3 9.6 10.3
-1 7 8 18.3 -18.2 1 7 2 35.4 -36.1 0 10 2 22.8 25.1
-1 7 11 5.9 -5.7 1 5 11 10.8 -11.5 0 8 13 5.1 -5.0
1 9 1 25.6 -27.2 1 5 10 7.4 -7.3 0 8 12 10.5 10.9
1 9 0 15.1 -15.8 1 5 7 26.3 -26.3 0 8 11 15.4 16.7
-1 9 1 67.8 -68.7 1 5 6 31.4 -30.4 0 8 9 15.2 -15.4
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0 8 8 7.0 -6.9 0 0 6 56.3 58.0 2 6 2 35.4 34.5
0 8 7 27.0 27.1 0 0 5 76.1 73.7 2 6 1 103.6 -103.7
0 8 6 32.5 31.9 0 0 4 73.9 77.1 2 6 0 121.9 122.4
0 8 4 13.0 -13.2 0 0 2 15.6 15.0 -2 6 1 50.3 46.3
0 8 2 26.2 27.1 0 0 1 73.1 -74.1 2 4 11 8.0 8.7
0 8 1 16.0 16.5 0 2 9 3.9 -3.9 2 4 10 9.9 11.2
0 6 14 17.2 15.4 -1 3 1 145.0 -145.3 2 4 8 5.3 -5.8
0 6 12 15.3 15.7 1 3 3 103.1 -102.7 2 4 7 16.6 16.6
0 6 11 46.7 -48.8 -1 3 8 4.5 4.5 2 4 6 33.4 32.6
0 6 10 42.6 44.4 -1 3 5 145.5 -145.2 2 4 5 7.5 7.2
0 6 9 7.2 -8.2 2 14 2 8.7 9.6 2 4 4 20.1 -19.9
0 6 8 68.6 67.8 2 14 1 13.0 13.9 2 4 2 58.4 55.4
0 6 7 70.4 -69.2 -2 14 1 9.5 -9.5 2 4 1 52.2 51.6
0 6 6 10.1 9.7 2 12 8 27.3 29.4 -2 4 1 27.9 -27.9
0 6 5 21.0 20.0 2 12 7 11.8 -11.7 2 2 13 8.0 -7.1
0 6 4 87.8 87.8 2 12 5 21.3 -21.9 2 2 11 22.0 22.2
0 6 3 51.7 -53.2 2 12 4 58.8 59.2 2 2 10 17.6 19.5
0 6 2 33.5 33.7 2 12 3 24.3 -23.5 2 2 8 24.4 -26.8
0 6 1 74.8 -74.8 2 12 2 17.8 18.7 2 2 7 5.9 5.4
0 4 12 17.1 16.8 2 12 1 51.5 -52.1 2 2 6 52.2 53.5
0 4 11 22.3 23.1 2 12 0 56.4 54.0 2 2 5 46.6 46.2
0 4 9 23.1 -25.9 -2 12 1 12.2 11.6 2 2 3 27.9 -27.5

0 4 8 11.0 -10.6 2 10 8 10.6 -11.0 2 2 1 34.5 35.1
0 4 7 39.7 40.9 2 10 6 23.9 23.6 2 2 0 45.6 48.0
0 4 6 55.6 55.3 2 10 5 12.1 12.0 -2 2 1 39.6 41.8
0 4 5 17.7 15.5 2 10 4 8.4 -8.7 2 0 15 21.0 -17.7
0 4 4 24.5 -24.4 2 10 3 10.7 -10.4 2 0 14 15.3 13.2
0 4 3 15.2 -14.7 2 10 2 15.0 15.6 2 0 12 51.8 47.7
0 4 2 27.3 29.5 2 10 1 19.3 18.9 2 0 11 49.3 -48.4
0 4 1 39.2 41.5 2 10 0 5.9 5.6 2 0 10 8.1 9.1
0 4 0 47.6 50.0 2 8 11 8.7 9.6 2 0 8 68.4 71.7
0 2 11 16.6 16.2 2 8 10 9.5 9.8 2 0 7 4.7 -4.8
0 2 10 11.3 10.7 2 8 8 8.3 -7.7 2 0 6 6.9 -6.4
0 2 8 4.3 4.3 2 8 7 6.9 7.1 2 0 5 60.4 -64.4
0 2 7 32.2 31.9 2 8 6 25.3 26.4 2 0 4 146.6 144.8
0 2 6 19.2 20.4 2 8 5 8.5 8.9 2 0 3 73.0 -69.0
0 2 5 11.6 -11.1 2 8 4 14.7 -14.8 2 0 2 128.3 125.8
0 2 3 60.8 60.2 2 8 2 26.7 27.0 2 0 1 119.5 -120.4
0 2 2 83.1 82.0 2 8 1 31.4 30.7 -2 0 1 18.5 19.3
0 2 1 8.7 8.7 -2 8 1 16.4 -16.9 -2 0 3 72.9 -69.9
0 2 0 35.8 -36.6 2 6 13 7.1 -7.3 -2 0 4 102.6 102.1
0 0 15 21.9 -21.4 2 6 12 40.9 43.1 -2 0 5 17.4 15.3
0 0 14 13.3 12.7 2 6 11 28.8 -31.2 -2 0 6 114.6 118.7
0 0 13 13.3 13.5 2 6 10 11.5 12.4 -2 0 7 134.8 -136.3
0 0 12 31.9 31.5 2 6 9 13.6 -13.3 -2 0 8 40.8 43.9
0 0 11 54.0 -50.5 2 6 8 45.7 42.7 -2 0 10 69.0 69.7
0 0 10 53.7 50.6 2 6 7 16.8 -16.1 -2 0 11 20.2 -20.1
0 0 9 35.8 -35.7 2 6 5 27.7 -25.6 -2 0 12 10.2 -9.4
0 0 8 73.5 75.0 2 6 4 117.3 117.2 -2 0 13 10.3 -10.4
0 0 7 71.1 -72.6 2 6 3 60.9 -58.5 -2 0 14 35.8 35.4
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-2 0 15 17.0 -15.2 -2 10 9 11.4 -11.0 3 7 5 16.7 -16.9
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-2 2 2 41.9 44.0 -2 10 12 11.7 11.6 3 7 8 7.6 7.8
-2 2 3 13.8 15.2 -2 12 2 11.1 12.4 3 7 10 9.9 -10.0
-2 2 4 23.3 -24.1 -2 12 3 45.4 -46.3 3 7 11 4.3 -4.3
-2 2 5 13.8 -15.3 -2 12 4 26.3 26.4 -3 9 1 94.3 -92.3
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-2 2 7 57.7 57.9 -2 12 7 47.7 -48.9 3 9 1 7.2 -6.8
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-2 2 11 10.7 11.3 -2 14 3 9.1 9.5 3 9 6 53.9 53.8
-2 2 12 24.9 25.0 -3 1 1 23.6 24.1 3 9 7 41.5 -40.4
-2 2 13 9.7 9.1 3 1 1 41.7 -41.5 3 9 9 35.2 -35.0
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-2 4 2 13.1 13.0 3 1 3 4.8 -4.8 -3 11 1 12.6 12.9
-2 4 3 48.7 48.6 3 1 5 17.4 -16.8 3 11 0 6.6 -6.4
-2 4 4 28.7 27.6 3 1 6 18.6 -19.3 3 11 1 22.1 -22.1
-2 4 7 19.6 19.2 3 1 9 11.0 -11.7 3 11 2 9.9 -10.2
-2 4 8 15.9 15.5 3 1 10 14.9 -15.8 3 11 3 8.4 7.9
-2 4 9 8.2 -7.8 -3 3 1 176.8 -177.3 3 11 4 10.0 9.7
-2 4 11 14.1 15.0 3 3 0 76.4 73.3 3 11 5 13.2 -12.1
-2 4 12 12.7 13.4 3 3 1 35.7 -33.4 3 11 6 14.0 -14.7
-2 4 14 9.9 -9.4 3 3 2 51.6 51.6 3 11 8 5.4 5.2
-2 6 2 25.1 24.7 3 3 3 85.7 -85.6 -3 13 1 10.1 10.7
-2 6 3 88.7 -89.0 3 3 4 19.1 -18.8 3 13 0 6.8 7.2
-2 6 4 40.0 37.9 3 3 5 9.9 -9.7 3 13 1 11.5 -11.2
-2 6 6 98.9 99.1 3 3 6 66.9 67.0 3 13 2 10.8 -10.9
-2 6 7 81.1 -78.0 3 3 7 67.7 -67.4 -3 13 6 11.6 11.5
-2 6 8 37.2 36.9 3 3 8 7.5 8.1 -3 13 5 8.0 8.3
-2 6 9 14.5 -14.1 3 3 9 40.7 -43.6 -3 13 4 9.2 -9.3
-2 6 10 44.2 41.2 3 3 10 44.5 47.9 -3 13 3 23.4 -23.0
-2 6 11 21.6 -21.6 3 3 11 16.0 -15.1 -3 11 10 5.7 5.9
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-2 6 15 18.3 -18.1 3 3 13 17.6 -15.3 -3 11 7 12.6 -12.0
-2 8 2 15.3 15.7 -3 5 1 26.6 28.2 -3 11 6 6.0 5.4
-2 8 3 26.8 27.4 3 5 0 9.5 10.4 -3 11 4 9.1 -8.9
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-2 8 5 7.1 -7.6 3 5 2 32.4 -33.9 -3 9 12 40.4 40.9
-2 8 7 21.2 21.4 3 5 5 12.7 -12.0 -3 9 11 24.4 -24.3
-2 8 8 10.7 11.2 3 5 6 12.3 -12.2 -3 9 9 53.2 -51.2
-2 8 9 9.6 -9.0 3 5 9 12.1 -11.9 -3 9 8 40.6 40.3
-2 8 11 9.3 9.4 3 5 10 13.3 -15.0 -3 9 5 51.4 -48.8
-2 8 12 13.4 13.2 3 5 12 9.6 9.7 -3 9 4 32.8 32.6
-2 10 2 11.5 11.5 -3 7 1 10.4 10.9 -3 9 3 26.7 -25.6
-2 10 3 14.7 15.9 3 7 0 8.8 -8.8 -3 9 2 32.0 32.0

-2 10 5 8.7 -8.9 3 7 1 34.2 -34.0 -3 7 14 7.4 7.2
-2 10 6 8.3 7.5 3 7 2 18.6 -17.5 -3 7 13 6.2 -5.7
-2 10 7 19.4 19.1 3 7 3 11.6 11.1 -3 7 12 11.6 -11.7
-2 10 8 13.6 11.4 3 7 4 7.7 7.8 -3 7 11 7.9 -7.7
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-3 7 10 8.9 8.5 -4 10 1 7.6 -7.6 4 0 0 23.9 24.5
-3 7 8 17.9 -16.9 4 8 10 11.8 11.4 -4 0 4 32.9 33.6
-3 7 7 16.4 -16.2 4 8 8 9.7 -9.1 -4 0 5 60.2 -57.6
-3 7 4 15.7 -15.3 4 8 7 8.6 -7.6 -4 0 6 115.1 115.3
-3 7 3 28.4 -28.9 4 8 6 12.5 13.0 -4 0 7 26.3 -26.8
-3 5 13 5.1 -5.1 4 8 5 24.8 24.7 -4 0 8 6.2 5.6
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-3 5 9 7.9 -8.3 4 8 1 19.3 18.4 -4 0 10 43.3 43.6
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-3 5 6 22.9 22.9 4 6 10 7.3 -6.6 -4 0 13 32.6 -31.4
-3 5 5 15.0 14.7 4 6 9 23.0 -21.2 -4 0 14 44.6 42.3
-3 5 4 28.7 -28.7 4 6 8 38.4 38.1 -4 2 2 20.8 -24.3
-3 5 3 59.4 -59.3 4 6 6 34.1 33.3 -4 2 3 17.6 18.7
-3 5 2 17.2 -16.3 4 6 5 72.5 -69.3 -4 2 4 35.6 37.3
-3 3 15 18.2 -16.0 4 6 4 58.2 57.2 -4 2 5 16.0 14.9
-3 3 14 7.6 -7.3 4 6 2 47.0 43.1 -4 2 8 17.4 16.5
-3 3 13 15.9 -16.0 4 6 1 49.2 -49.4 -4 2 11 8.7 8.7
-3 3 12 46.2 49.0 4 6 0 26.6 26.5 -4 2 12 14.7 15.6
-3 3 11 39.8 -43.0 -4 6 1 14.6 14.6 -4 2 13 7.0 6.8
-3 3 10 7.9 8.1 4 4 10 15.1 15.0 -4 2 14 8.2 -8.3
-3 3 9 67.6 -66.9 4 4 9 8.8 8.7 -4 2 15 7.6 -7.5
-3 3 8 69.6 67.9 4 4 8 10.3 -11.6 -4 4 2 7.9 8.1
-3 3 7 11.0 -10.4 4 4 7 12.8 -11.9 -4 4 3 23.7 24.5
-3 3 6 20.1 -18.7 4 4 6 15.2 16.4 -4 4 4 15.0 14.9
-3 3 5 86.0 -86.4 4 4 5 32.7 31.9 -4 4 5 14.6 -14.1
-3 3 4 55.0 54.0 4 4 4 14.4 13.2 -4 4 7 20.0 18.5
-3 3 3 34.1 -33.9 4 4 3 14.3 -14.8 -4 4 8 33.8 33.4
-3 3 2 75.0 73.3 4 4 1 20.4 20.2 -4 4 10 16.3 -16.5
-3 1 16 8.6 -7.4 4 4 0 20.4 20.8 -4 4 11 4.7 -4.7
-3 1 13 6.9 -6.5 -4 4 1 6.2 5.6 -4 4 12 12.3 12.5
-3 1 12 9.9 -10.1 4 2 10 6.9 7.5 -4 4 13 12.3 13.4

-3 1 11 5.2 -5.0 4 2 6 23.5 24.4 -4 4 15 6.7 -6.3
-3 1 9 6.1 -6.4 4 2 5 24.1 24.4 -4 6 2 68.8 66.8
-3 1 8 31.2 -33.1 4 2 4 10.0 -9.0 -4 6 3 86.5 -83.2
-3 1 7 18.6 -18.4 4 2 3 24.3 -25.0 -4 6 4 38.1 37.0
-3 1 6 16.8 17.0 4 2 2 15.7 14.7 -4 6 5 20.3 -21.4
-3 1 5 11.8 11.7 4 2 1 49.7 52.7 -4 6 6 95.0 93.2
-3 1 4 34.7 -33.9 4 2 0 31.9 35.6 -4 6 7 36.2 -35.6
-3 1 3 67.4 -67.1 -4 2 1 13.3 -15.9 -4 6 8 12.0 -11.4
-3 1 2 13.7 -15.5 4 0 13 20.9 -17.7 -4 6 9 18.6 -18.3
4 12 4 34.6 35.8 4 0 12 34.1 30.8 -4 6 10 46.6 45.8
4 12 2 19.4 20.2 4 0 9 20.1 -20.2 -4 6 12 11.3 10.9
4 12 1 34.9 -36.0 4 0 8 34.4 38.8 -4 6 13 32.4 -33.6
4 12 0 14.6 15.3 4 0 7 12.5 -13.6 -4 6 14 27.5 29.0
4 10 6 10.3 10.7 4 0 6 34.9 37.3 -4 8 3 17.0 17.0
4 10 5 12.9 12.9 4 0 5 72.0 -74.9 -4 8 4 12.4 12.2
4 10 3 11.9 -11.9 4 0 4 99.4 96.6 -4 8 5 5.4 -5.5
4 10 1 19.4 19.3 4 0 2 39.7 37.7 -4 8 6 5.6 -5.6
4 10 0 12.3 12.5 4 0 1 83.0 -86.1 -4 8 7 10.9 10.9
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-4 8 8 23.1 23.1 5 9 1 17.8 -18.4 -5 1 9 16.9 -17.9
-4 8 10 10.9 -11.1 5 9 2 23.5 22.7 -5 1 8 20.2 -21.1
-4 8 12 10.6 10.1 5 9 3 58.7 -56.5 -5 1 6 13.8 13.8
-4 10 3 10.6 11.4 5 9 4 21.6 21.3 -5 1 5 5.2 -5.1
-4 10 4 16.2 16.3 5 9 6 11.0 11.1 -5 1 4 32.7 -32.6
-4 10 8 13.0 13.5 5 9 7 28.4 -28.4 -5 1 3 19.2 -21.1
-4 10 10 5.8 -6.2 -5 11 1 10.2 9.9 6 10 2 8.1 -8.3
-4 12 2 41.8 41.5 5 11 1 13.9 -13.2 6 10 0 13.4 13.3
-4 12 3 47.7 -47.8 -5 11 7 7.8 7.2 6 8 5 11.8 12.2
-4 12 4 13.3 14.4 -5 11 6 12.5 12.9 6 8 4 8.2 7.8
-4 12 5 15.9 -17.4 -5 11 4 20.0 -19.9 6 8 3 9.8 -9.5
-4 12 6 50.3 52.4 -5 11 3 14.3 -14.6 6 8 1 11.8 11.5
-4 12 7 18.3 -19.4 -5 11 2 10.4 11.4 6 8 0 22.2 19.9
5 1 0 15.8 -18.2 -5 9 9 17.5 -17.3 -6 8 1 4.6 4.5
5 1 1 25.3 -25.4 -5 9 8 47.6 46.6 6 6 7 9.5 -9.6
5 1 4 11.3 -11.0 -5 9 7 45.8 -45.0 6 6 6 34.9 33.0
5 1 5 18.0 -17.9 -5 9 5 26.3 -25.2 6 6 5 34.3 -34.1
5 1 6 4.3 -4.3 -5 9 4 45.2 45.2 6 6 4 10.5 10.4

5 1 7 7.7 8.0 -5 9 3 11.7 -12.5 6 6 2 43.9 40.5
5 1 9 11.0 -12.5 -5 9 2 10.8 -10.7 6 6 1 37.5 -35.1
5 1 10 7.9 -7.7 -5 7 9 17.5 -17.3 6 6 0 6.9 7.4
-5 3 1 64.9 -66.0 -5 7 8 12.5 -12.6 -6 6 1 28.4 -27.8
5 3 0 77.7 81.8 -5 7 7 7.2 6.8 6 4 6 5.9 5.9
5 3 1 36.3 -37.4 -5 7 6 15.8 16.0 6 4 5 17.0 16.8
5 3 2 20.3 21.1 -5 7 5 6.6 -6.3 6 4 4 8.4 8.7
5 3 3 90.0 -90.2 -5 7 4 29.4 -30.5 6 4 3 12.9 -12.2
5 3 4 35.8 33.8 -5 7 3 19.8 -18.8 6 4 2 12.7 -11.8
5 3 5 11.3 10.6 -5 7 2 12.3 12.9 6 4 1 17.8 17.0
5 3 6 16.0 16.3 -5 5 13 11.8 -11.9 6 4 0 28.9 29.5
5 3 7 44.3 -43.4 -5 5 10 10.9 10.0 -6 4 1 7.5 7.8
5 3 9 10.2 -11.6 -5 5 9 12.6 -12.5 6 2 9 10.9 11.5
5 3 10 29.8 32.2 -5 5 8 20.5 -20.5 6 2 7 9.5 -9.5
5 3 11 28.2 -28.4 -5 5 6 9.8 10.0 6 2 5 15.6 15.4
5 5 0 19.2 -18.9 -5 5 4 21.6 -22.1 6 2 4 18.6 17.9
5 5 1 18.4 -18.4 -5 5 3 15.6 -15.6 6 2 2 8.6 -8.7
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5 5 4 11.8 -11.1 -5 3 14 5.6 5.3 6 0 9 35.3 -37.0
5 5 5 20.0 -19.5 -5 3 13 6.5 6.9 6 0 8 20.4 23.4
5 5 7 9.0 8.7 -5 3 12 22.1 22.9 6 0 6 48.4 48.0
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