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Cation ordering in synthetic and natural Ni–Mg olivine

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Abstract

The crystal structures of natural liebenbergite—$(Ni_{1.52}Co_{0.05}Fe_{0.09}Mg_{0.34})SiO_4$—from Barberton, South Africa, and of synthetic liebenbergite—$(Ni_{1.16}Mg_{0.84})SiO_4$—synthesized at 500°C, have been studied in order to determine the intracrystalline Ni–Mg distribution. The natural liebenbergite is fully ordered, with M1 occupied only by Ni, whereas the synthetic sample is only partially ordered with $K_D = [Mg(M2) \cdot Ni(M1)]/[Ni(M2) \cdot Mg(M1)] = 9.9(4)$, $\Delta G^\circ_{ex} = -3.5$ kcal/mole. Comparison with the results of Rajamani *et al.* (1975), who found $K_D = 9.2(2)$ and $\Delta G^\circ_{ex} = -6.9$ kcal/mole for a sample synthesized at 1280°C, implies that the 500°C synthetic sample in the present study crystallized metastably in a disordered or partially ordered state and ordering proceeded slowly.

Although site size effects are small in Fe–Mg, Ni–Mg, and Co–Mg olivines, the crystal field stabilization energy is important in determining the observed cation distribution in Ni–Mg and Co–Mg olivines. Electronegativity or covalency effects are known only qualitatively, but there is a preference of less electronegative ions (Mg, Ca) for M2.

Ordering of Ni into the M1 site of olivine should appreciably affect Ni partitioning between olivine and melt, and activity–composition relations have been examined assuming ideal solution behavior. Deviations from Raoult's law increase with increasing order, but variations in activity coefficients are less than 10 percent below 10 mole% Ni.

Introduction

Although nickel is a common and important minor constituent in olivines, liebenbergite, the nickel-rich olivine, has been found only in the unusual Bon Accord deposit in Barberton, South Africa. The material at Bon Accord originally filled interstices between trevorite grains in the assemblage trevorite–nickel serpentine–nickel ludwigite–bunsenite–violarite–millerite–gaspeite–nimite but is now almost completely replaced by secondary nickel serpentine. Only small irregular crystals remain in the serpentine matrix (de Waal and Calk, 1973). The liebenbergite appears to have formed at about 730°C and less than 2 kbar during thermal metamorphism, possibly of a nickel-rich meteorite (de Waal, 1978). I have obtained crystals of liebenbergite through the courtesy of Dr. de Waal.

The natural occurrence of liebenbergite presents us with the unique opportunity to examine a mineral that previously had been studied in synthetic form only (*e.g.* Rajamani *et al.*, 1975). The natural sample equilibrated over a long period at a fairly low temperature (730°C), so it should possess an equilibrium distribution of cations. Typical synthesis experiments are of short duration at high temperature. For example, the Ni–Mg olivine examined by Rajamani *et al.* (1975) was crystallized at 1280°C and cooled in several days yielding a zoned crystal. The authors questioned whether the observed K_D, $[Mg(M2) \cdot Ni(M1)]/[Ni(M2) \cdot Mg(M1)]$, represented an equilibrium distribution of cations.

During a study of hydrous nickel–magnesium silicates (Brindley *et al.*, 1979), euhedral crystals of liebenbergite were synthesized by reacting natural pimelite (nickel–magnesium talc) at 500°C and 2.1 kbar for 4 weeks. These crystals should differ significantly from the products of short-term reactions at temperatures in excess of 1200°C.

Numerous studies have focused on the nature and causes of intracrystalline cation distributions in natural and synthetic olivines (see Rajamani *et al.*, 1975, for a summary). In an attempt to understand order-

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APPENDIX A

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR Ni-Mg OLIVINE (Synthetic)

h= 0,k= 0

ℓ	F_O	F_C
2	16	16
6	17	17
8	75	75
10	13	13

h= 0,k= 2

ℓ	F_O	F_C
0	62	61
1	44	41
2	71	71
3	5	5
4	43	40
5	33	31
6	50	47
7	3	2
8	26	25
9	18	17
10	29	27
11	1	1

h= 0,k= 4

ℓ	F_O	F_C
0	60	58
1	46	44
2	49	47
3	60	56
4	53	49
5	22	20
6	36	34
7	36	34
8	32	29
9	9	9
10	24	22
11	18	17

h= 0,k= 6

ℓ	F_O	F_C
0	21	20
1	71	68
3	55	53
4	7	6

h= 0,k= 6

ℓ	F_O	F_C
5	45	43
6	87	82
7	29	27
8	4	4
9	25	23
10	41	39

h= 0,k= 8

ℓ	F_O	F_C
0	50	48
1	6	6
2	47	45
3	18	18
4	41	40
5	4	3
6	33	31
7	16	15
8	27	26
9	4	3
10	22	21

h- 0,k=10

ℓ	F_O	F_C
0	56	54
1	44	42
2	12	12
3	29	28
4	48	46
5	37	36
6	13	12
7	14	14
8	33	33
9	23	22

h= 0,k=12

ℓ	F_O	F_C
0	57	58
1	46	46
2	39	39
3	45	45
4	45	45

h= 0,k=12

ℓ	F_O	F_C
5	33	32
6	23	23
7	32	32
8	25	25

h=0,k=14

ℓ	F_O	F_C
0	29	32
1	13	13
2	24	24
3	5	5
4	28	28
5	15	16
6	19	20
7	0	1

h= 0,k=16

ℓ	F_O	F_C
0	8	10
1	11	13
2	44	44
3	15	17
4	6	7
5	7	7
6	37	38

h= 0,k=18

ℓ	F_O	F_C
0	39	41
1	18	19
2	17	17
3	14	14
4	34	35

h= 1,k= 0

ℓ	F_O	F_C
1	23	26
3	7	7
5	21	25
7	5	6
9	12	13
11	3	3

h= 1,k= 1

ℓ	F_O	F_C
0	38	40
1	36	37
3	32	33
4	30	28
5	17	18
6	59	62
7	15	15
8	14	15
9	7	8
10	30	32
11	7	8

h= 1,k= 2

ℓ	F_O	F_C
0	26	25
1	16	15
2	52	49
3	24	22
4	8	9
5	3	2
6	7	8
7	13	12
8	2	2
9	0	0
10	2	1
11	6	6

h= 1,k= 3

ℓ	F_O	F_C
1	74	75
2	55	53
3	63	61
4	80	78
5	49	47
6	28	26
7	34	32
8	41	38
9	24	23
10	15	14
11	16	15

h= 1,k= 4

ℓ	F_O	F_C
0	63	57
1	0	1
2	6	6
3	11	10
4	24	23
5	10	10
6	2	2
7	6	6
8	5	5
9	7	6
10	7	7

h= 1,k= 5

ℓ	F_O	F_C
0	67	64
1	33	31
2	68	66
3	24	23
4	51	48
5	20	19
6	39	37
7	12	11
8	29	28
9	10	10
10	22	21

h= 1,k= 6

ℓ	F_O	F_C
0	17	16
1	1	1
2	6	6
3	18	17
4	10	10
5	8	8
6	5	4
7	15	14
8	5	4
9	7	6
10	3	3

h= 1,k= 7

ℓ	F_O	F_C
0	108	107
1	5	4
2	6	6
3	7	7
4	85	81
5	3	2
6	5	5
7	6	5
8	49	46
9	1	1
10	6	5

h= 1,k= 8

ℓ	F_O	F_C
0	14	13
1	12	12
2	25	25
3	6	5
4	4	4
5	11	10
6	10	10
7	2	2
8	4	3
9	7	6
10	2	1

h= 1,k= 9

ℓ	F_O	F_C
0	10	9
1	24	23
2	90	87
3	23	22
4	8	7
5	17	16
6	58	56
7	14	14
8	6	5
9	9	8

h= 1,k=10

ℓ	F_O	F_C
0	8	8
1	8	8
2	14	13
3	1	1
4	4	4
5	11	11
6	5	5
7	3	3
8	2	2
9	9	9

h= 1,k=11

ℓ	F_O	F_C
0	49	48
1	4	0
2	30	29
3	2	1
4	40	39
5	1	0
6	22	21
7	2	1
8	27	26
9	1	0

h=1,k=12

ℓ	F_O	F_C
0	2	2
1	1	0
2	9	10
3	8	8
4	2	2
5	6	6
6	6	6
7	10	10
8	2	2

h=1,k=13

ℓ	F_O	F_C
0	9	10
1	26	26
2	51	51
3	22	22
4	9	9
5	21	21
6	38	38
7	14	14
8	8	8

h= 1,k=14

ℓ	F_O	F_C
0	19	19
1	2	2
2	2	2
3	2	0
4	13	14
5	2	2
6	3	2
7	2	1

h= 1,k=15

ℓ	F_O	F_C
0	50	52
1	4	4
2	6	6
3	5	5
4	43	44
5	3	2
6	6	5
7	4	4

h= 1,k=16

ℓ	F_O	F_C
0	2	3
1	2	2
2	7	8
3	7	7
4	1	1
5	3	2
6	3	4

h= 1,k=17

ℓ	F_O	F_C
0	23	24
1	7	8
2	20	22
3	7	8
4	21	22
5	6	6

h= 1,k=18

ℓ	F_O	F_C
0	4	4
1	5	5
2	4	4
3	1	0

h= 1,k=19

ℓ	F_O	F_C
0	18	19
1	19	21

h= 2,k= 0

ℓ	F_O	F_C
0	54	70
2	6	7
4	57	69
6	9	10
8	37	44
10	12	14

h= 2,k= 1

ℓ	F_O	F_C
0	31	33
1	32	35
2	10	12
3	22	24
4	18	20
5	21	23
6	10	10
7	12	12
8	8	8
9	11	12
10	6	7

h= 2,k= 2

ℓ	F_O	F_C
0	31	32
1	9	7
3	13	13
4	20	21
5	11	11
6	63	66
7	12	11
8	9	9
9	8	7
10	31	33

h= 2,k= 3

ℓ	F_O	F_C
0	21	21
1	2	2
2	18	18
3	4	3
4	17	17
5	5	5
6	12	12
7	3	3
8	9	9
9	3	3
10	6	6

h= 2,k= 4

ℓ	F_O	F_C
1	47	47
2	49	49
3	26	26
4	77	76
5	38	37
6	26	26
7	11	11
8	38	37
9	20	20
10	11	11

h= 2,k= 5

ℓ	F_O	F_C
0	5	5
1	31	30
2	11	10
3	29	29
4	0	0
5	20	19
6	4	4
7	18	17
8	2	2
9	10	10
10	2	0

h= 2,k= 6

ℓ	F_O	F_C
0	14	13
1	23	22
2	58	56
3	22	21
4	15	14
5	16	15
6	45	43
7	13	12
8	16	16
9	8	7
10	30	29

h= 2,k= 7

ℓ	F_O	F_C
0	20	20
1	12	12
2	29	28
3	14	14
4	17	17
5	7	7
6	17	16
7	10	9
8	11	11
9	4	3
10	8	7

h= 2,k= 8

ℓ	F_O	F_C
0	74	74
1	25	24
2	34	33
3	33	32
4	57	55
5	8	8
6	21	20
7	25	24
8	33	32
9	3	3

h= 2,k= 9

ℓ	F_O	F_C
0	16	16
1	4	4
2	18	18
3	7	7
4	13	13
5	2	1
6	13	11
7	6	5
8	8	8
9	1	0

h= 2,k=10

ℓ	F_O	F_C
0	65	63
1	29	28
2	37	36
3	33	31
4	51	49
5	17	16
6	23	22
7	23	22
8	28	28
9	9	8

h= 2,k=11

ℓ	F_O	F_C
0	1	1
1	19	18
2	9	9
3	16	15
4	2	2
5	15	14
6	4	5
7	10	9
8	3	3

h= 2,k=12

ℓ	F_O	F_C
0	23	23
1	21	20
2	23	22
3	16	16
4	22	22
5	16	16
6	21	21
7	10	9
8	21	20

h= 2,k=13

ℓ	F_O	F_C
0	18	18
1	1	1
2	13	13
3	1	1
4	15	15
5	2	2
6	10	10
7	2	2

h= 2,k=14

ℓ	F_O	F_C
0	38	38
1	19	18
2	21	21
3	10	10
4	33	33
5	22	21
6	15	15
7	5	4

h= 2,k=15

ℓ	F_O	F_C
0	11	11
1	8	8
2	9	9
3	5	6
4	9	10
5	8	8
6	7	7

h= 2,k=16

ℓ	F_O	F_C
0	12	13
1	6	6
2	47	48
3	3	2
4	10	10
5	7	8

h= 2,k=17

ℓ	F_O	F_C
0	8	9
1	7	8
2	3	3
3	7	7
4	6	7

h= 2,k=18

ℓ	F_O	F_C
0	20	22
1	6	7
2	7	7
3	7	8

h= 3,k= 0

ℓ	F_O	F_C
1	17	20
3	29	33
5	6	6
7	21	24
9	2	1

h= 3,k= 1

ℓ	F_O	F_C
0	56	62
1	30	33
2	61	70
3	20	22
4	38	43
5	22	25
6	36	41
7	9	10
8	21	23
9	12	13
10	19	22

h= 3,k= 2

ℓ	F_O	F_C
0	26	27
1	15	16
2	57	63
3	8	8
4	24	26
5	14	15
6	29	31
7	3	3
8	18	20
9	8	8
10	11	12

h= 3,k= 3

ℓ	F_O	F_C
0	66	70
1	46	48
2	23	24
3	40	41
4	53	55
5	30	31
6	19	19
7	22	23
8	33	34
9	15	17
10	13	14

h= 3,k= 4

ℓ	F_O	F_C
0	50	52
1	32	32
2	18	17
3	34	35
4	33	34
5	17	18
6	16	16
7	22	22
8	14	14
9	9	9
10	13	13

h= 3,k= 5

ℓ	F_O	F_C
0	39	40
1	15	15
2	68	68
3	19	19
4	31	30
5	6	6
6	42	42
7	13	13
8	17	17
9	3	2
10	23	23

h= 3,k= 6

ℓ	F_O	F_C
0	2	2
1	29	28
2	4	4
3	14	14
4	0	0
5	29	28
6	3	2
7	5	5
8	1	1
9	18	17
10	2	0

h= 3,k= 7

ℓ	F_O	F_C
0	79	79
1	10	10
2	23	23
3	12	12
4	62	61
5	4	4
6	15	14
7	9	8
8	36	35
9	3	2

h= 3,k= 8

ℓ	F_O	F_C
0	47	46
1	6	5
2	20	18
3	2	2
4	35	34
5	6	6
6	17	17
7	1	0
8	17	16
9	4	4

h= 3,k= 9

ℓ	F_O	F_C
0	2	2
1	9	9
2	63	62
3	8	8
4	4	3
5	8	7
6	47	46
7	5	5
8	5	5
9	4	4

h= 3,k=10

ℓ	F_O	F_C
0	1	1
1	32	31
2	16	15
3	23	23
4	2	2
5	28	27
6	8	8
7	13	13
8	5	4

h= 3,k=11

ℓ	F_O	F_C
0	49	48
1	3	3
2	21	21
3	7	7
4	40	40
5	2	1
6	16	16
7	7	7
8	27	26

h= 3,k=12

ℓ	F_O	F_C
0	11	11
1	18	18
2	4	5
3	23	23
4	8	9
5	8	8
6	5	4
7	20	20
8	4	5

h= 3,k=13

ℓ	F_O	F_C
0	15	15
1	9	9
2	47	48
3	10	10
4	12	12
5	5	6
6	36	35
7	8	7

h= 3,k=14

ℓ	F_O	F_C
0	6	6
1	8	8
2	22	23
3	8	9
4	7	7
5	6	6
6	14	14

h= 3,k=15

ℓ	F_O	F_C
0	35	36
1	11	11
2	6	6
3	10	10
4	32	33
5	9	9
6	6	7

h= 3,k=16

ℓ	F_O	F_C
0	1	1
1	15	15
2	8	8
3	18	19
4	1	1
5	9	9

h= 3,k=17

ℓ	F_O	F_C
0	20	20
1	9	9
2	21	22
3	6	6

h= 3,k=1°

ℓ	F_O	F_C
0	8	9
1	11	12

h= 4,k= 0

ℓ	F_O	F_C
2	22	23
4	70	78
6	10	11
8	37	41
10	3	3

h= 4,k= 1

ℓ	F_O	F_C
0	10	11
1	8	8
2	26	28
3	10	11
4	11	11
5	5	5
6	14	15
7	7	8
8	9	9
9	3	1
10	5	5

h= 4,k= 2

ℓ	F_O	F_C
0	17	19
1	9	10
2	56	62
3	16	17
4	15	17
5	1	1
6	38	42
7	12	13
8	13	14
9	1	1
10	25	27

h= 4,k= 3

ℓ	F_O	F_C
0	17	18
1	2	2
2	17	19
3	8	9
4	15	15
5	4	4
6	12	12
7	8	8
8	9	8
9	4	3

h= 4,k= 4

ℓ	F_O	F_C
0	59	61
1	9	9
2	13	14
3	15	16
4	49	50
5	2	1
6	12	13
7	12	13
8	32	33
9	3	1

h= 4,k= 5

ℓ	F_O	F_C
0	23	23
1	22	22
2	6	5
3	18	18
4	17	16
5	18	18
6	6	6
7	10	10
8	7	7
9	10	10

h= 4,k= 6

ℓ	F_O	F_C
0	34	35
1	26	27
2	67	68
3	22	22
4	26	26
5	20	20
6	42	42
7	13	13
8	12	12
9	13	13

h= 4,k= 7

ℓ	F_O	F_C
0	21	20
1	2	2
2	7	7
3	2	2
4	15	15
5	4	3
6	8	7
7	3	3
8	5	6
9	2	2

h= 4,k= 8

ℓ	F_O	F_C
0	36	36
1	21	21
2	30	29
3	12	12
4	31	30
5	20	20
6	23	23
7	4	4
8	22	22

h= 4,k= 9

ℓ	F_O	F_C
0	13	13
1	10	10
2	10	9
3	4	3
4	11	10
5	12	11
6	8	7
7	1	0
8	5	6

h= 4,k=10

ℓ	F_O	F_C
0	21	21
1	20	20
2	28	28
3	13	13
4	20	20
5	20	20
6	24	23
7	7	6
8	17	17

h= 4,k=11

ℓ	F_O	F_C
0	7	7
1	20	20
2	6	5
3	19	19
4	5	5
5	15	15
6	2	2
7	13	13

h= 4,k=12

ℓ	F_O	F_C
0	29	29
1	19	19
2	40	40
3	20	20
4	23	23
5	14	14
6	28	28
7	16	16

h= 4,k=13

ℓ	F_O	F_C
0	2	2
1	2	1
2	9	9
3	2	2
4	2	2
5	3	3
6	4	4

h= 4,k=14

ℓ	F_O	F_C
0	30	31
1	6	6
2	14	14
3	10	10
4	28	28
5	2	2

h= 4,k=15

ℓ	F_O	F_C
0	2	2
1	6	6
2	6	6
3	9	9
4	2	2
5	2	1

h= 4,k=16

ℓ	F_O	F_C
0	7	7
1	9	9
2	23	24
3	12	12

h= 4,k=17

ℓ	F_O	F_C
0	3	3
1	10	10

h= 5,k= 0

ℓ	F_O	F_C
1	9	8
3	2	1
5	10	10
7	3	2
9	7	6

h= 5,k= 1

ℓ	F_O	F_C
0	39	40
1	33	34
2	26	27
3	35	36
4	32	34
5	20	20
6	20	21
7	25	26
8	23	24
9	10	11

h= 5,k= 2

ℓ	F_O	F_C
0	16	17
1	12	12
2	2	1
3	14	14
4	11	11
5	6	6
6	3	2
7	10	11
8	3	3
9	3	3

h= 5,k= 3

ℓ	F_O	F_C
0	50	52
1	3	2
2	39	41
3	3	3
4	38	40
5	2	2
6	24	26
7	3	2
8	21	23
9	1	1

h= 5,k= 4

ℓ	F_O	F_C
0	9	10
1	11	12
2	5	5
3	6	6
4	6	6
5	11	12
6	0	0
7	2	2
8	2	2
9	7	7

h= 5,k= 5

ℓ	F_O	F_C
0	0	2
1	25	26
2	58	60
3	17	17
4	3	3
5	22	23
6	42	44
7	10	9
8	5	5

h= 5,k= 6

ℓ	F_O	F_C
0	2	3
1	4	4
2	4	0
3	9	9
4	3	2
5	1	2
6	1	1
7	8	8
8	1	1

h= 5,k= 7

ℓ	F_O	F_C
0	38	39
1	19	19
2	14	14
3	13	13
4	34	34
5	18	18
6	13	13
7	6	6
8	25	26

h= 5,k= 8

ℓ	F_O	F_C
0	6	6
1	5	5
2	19	20
3	3	3
4	7	6
5	6	6
6	11	11
7	2	1
8	7	7

h= 5,k= 9

ℓ	F_O	F_C
0	30	32
1	9	9
2	39	40
3	7	6
4	25	26
5	8	8
6	27	27
7	3	3

h= 5,k=10

ℓ	F_O	F_C
0	1	2
1	2	2
2	8	8
3	5	5
4	0	0
5	3	2
6	5	4
7	5	5

h= 5,k=11

ℓ	F_O	F_C
0	55	55
1	3	3
2	6	6
3	3	2
4	47	48
5	5	6
6	3	3

h= 5,k=12

ℓ	F_O	F_C
0	3	0
1	4	4
2	4	4
3	0	1
4	1	0
5	7	6
6	3	2

h= 5,k=13

ℓ	F_O	F_C
0	9	9
1	0	1
2	26	26
3	3	3
4	10	10
5	4	3

h= 5,k=14

ℓ	F_O	F_C
0	15	15
1	4	4

h= 5,k=14

ℓ	F_O	F_C
2	4	4
3	2	3
4	11	12

h= 5,k=15

0	24	25
1	9	10
2	23	25
3	10	11

h= 5,k=16

0	3	4

h= 6,k= 0

0	21	20
2	30	29
4	19	18
6	25	24
8	16	16

h= 6,k= 1

0	18	18
1	13	13
2	2	2
3	8	8
4	14	13
5	14	13
6	4	5
7	4	4
8	6	5

h= 6,k= 2

0	8	7
1	24	24
2	58	58
3	18	17
4	7	6
5	22	22
6	42	42
7	10	10
8	4	4

h= 6,k= 3

0	0	0
1	2	2

h= 6,k= 3

ℓ	F_O	F_C
2	1	2
3	8	8
4	2	0
5	3	3
6	2	1
7	8	8
8	1	1

h= 6,k= 4

0	60	61
1	2	1
2	6	6
3	5	4
4	50	51
5	2	2
6	4	4
7	4	4
8	33	33

h= 6,k= 5

0	7	7
1	13	13
2	8	8
3	14	15
4	5	4
5	8	8
6	3	3
7	12	12

h= 6,k= 6

0	30	30
1	5	4
2	14	14
3	4	4
4	27	28
5	3	3
6	13	13
7	3	3

h= 6,k= 7

0	6	6
1	2	2
2	18	18
3	6	6
4	7	7
5	2	1

h= 6,k= 7

ℓ	F_O	F_C
6	11	11
7	7	7

h= 6,k= 8

0	33	34
1	29	30
2	20	20
3	31	32
4	29	30
5	21	21
6	14	15
7	24	25

h= 6,k= 9

0	4	4
1	7	7
2	7	7
3	0	1
4	4	4
5	9	9
6	6	5

h= 6,k=10

0	15	15
1	7	7
2	37	38
3	9	9
4	12	13
5	5	4
6	28	28

h= 6,k=11

0	3	3
1	8	8
2	10	10
3	6	6
4	1	1
5	8	8

h= 6,k=12

0	4	5
1	1	1
2	28	28
3	2	1
4	6	6

h= 6,k=13

ℓ	F_O	F_C
0	12	12
1	3	2
2	4	4
3	5	6

h= 6,k=14

0	30	30
1	22	22
2	9	9

h= 7,k= 0

1	6	6
3	3	2
5	8	7
7	3	1

h= 7,k= 1

0	43	40
1	20	19
2	20	19
3	13	12
4	36	34
5	20	19
6	14	14
7	6	6

h= 7,k= 2

0	2	1
1	6	6
2	8	8
3	5	4
4	2	2
5	6	5
6	5	5
7	3	3

h= 7,k= 3

0	24	23
1	7	7
2	11	10
3	7	7
4	24	22
5	6	6
6	12	11

h= 7,k= 4

ℓ	F_O	F_C
0	2	3
1	6	6
2	4	4
3	7	7
4	2	2
5	4	4
6	1	1

h= 7,k= 5

0	9	9
1	5	5
2	45	43
3	11	10
4	8	8
5	1	1
6	33	32

h= 7,k= 6

0	5	5
1	0	1
2	4	4
3	4	4
4	4	4
5	2	2
6	4	3

h= 7,k= 7

0	31	31
1	14	14
2	24	23
3	18	17
4	27	26
5	9	8

h= 7,k= 8

0	10	10
1	1	0
2	4	3
3	1	1
4	8	8
5	0	0

h= 7,k= 9

0	3	3
1	4	4

h= 7,k= 9

ℓ	F_O	F_C
2	25	25
3	5	4
4	4	4

h= 7,k=10

0	6	6
1	4	3
2	2	1
3	2	2
4	5	5

h= 7,k=11

0	34	34
1	4	4
2	7	8
3	8	9

h= 7,k=12

0	2	3
1	3	2

h= 8,k= 0

0	32	29
2	20	17
4	28	25

h= 8,k= 1

0	6	5
1	14	13
2	8	8
3	11	10
4	4	3
5	14	13

h= 8,k= 2

0	9	8
1	9	8
2	35	31
3	10	9
4	9	7
5	6	5

h= 8,k= 3

0	12	10
1	4	3

h= 8,k= 3

ℓ	F_o	F_c
2	10	9
3	3	3
4	10	9

h= 8,k= 4

0	35	31
1	2	2
2	7	7
3	4	3
4	31	28

h= 8,k= 5

0	14	13
1	5	5
2	2	1
3	7	6
4	11	10

h= 8,k= 6

0	22	20
1	7	6
2	24	22
3	6	6

h= 8,k= 7

0	3	1
1	11	11
2	13	12
3	14	13

h= 8,k= 8

0	22	20
1	15	14
2	15	15

h= 9,k= 1

0	18	15

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	0	6	23.591	22.582	-22.629	0.962	1.009	5.1800	0.9941	8
0	0	8	91.472	86.074	88.714	6.594	5.399	27.0112	0.9362	10
0	0	10	18.215	16.853	-16.852	0.821	1.362	4.5890	0.9977	12
0	2	1	35.157	34.749	-35.176	0.550	0.408	5.0609	0.9756	14
0	2	3	0.913 *	0.701	0.404	-0.573	0.212	0.3092	1.0000	16 * *
0	2	4	33.909	34.865	35.017	1.664	-0.956	-7.2684	0.9891	17
0	2	5	27.464	28.145	-28.226	0.484	-0.681	-4.5467	0.9939	18
0	2	6	60.431	60.867	61.342	6.369	-0.436	-2.6675	0.9741	19
0	2	7	2.571	1.129	-1.002	-0.520	1.442	2.8326	1.0000	20
0	2	8	22.896	22.160	22.156	1.530	0.736	3.4557	0.9956	21
0	2	9	15.965	15.545	-15.556	0.414	0.420	1.7507	0.9979	22
0	2	10	38.866	35.787	35.581	5.397	3.079	13.5868	0.9889	23
0	4	0	77.047	77.885	82.348	6.401	-0.838	-6.0703	0.8892	24
0	4	1	53.277	53.327	-54.370	-1.922	-0.050	-0.5285	0.9608	25
0	4	2	39.953	41.446	41.751	2.150	-1.493	-14.0970	0.9829	26
0	4	4	63.133	65.265	66.002	6.149	-2.132	-15.8579	0.9694	28
0	4	5	26.354	26.348	-26.351	-1.732	0.006	0.0400	0.9954	29
0	4	6	30.930	31.450	31.478	2.027	-0.520	-3.1086	0.9941	30
0	4	7	38.817	38.702	38.828	1.797	0.115	0.6320	0.9914	31
0	4	8	39.712	39.081	38.893	5.444	0.631	3.1587	0.9903	32
0	4	9	12.945	12.261	-12.182	-1.449	0.684	2.7079	0.9988	33
0	4	10	22.381	21.223	21.192	1.785	1.158	4.7901	0.9959	34
0	6	0	18.500	18.120	18.024	2.215	0.381	3.0906	0.9956	35
0	6	1	77.750	76.728	79.058	2.505	1.022	9.1803	0.9410	36
0	6	2	156.376	156.717	173.343	6.350	-0.341	-1.3259	0.8163	37
0	6	3	60.588	61.549	-62.294	-2.398	-0.961	-7.5305	0.9748	38
0	6	4	4.994	5.259	4.816	2.114	-0.265	-1.2071	0.9998	39
0	6	5	49.771	50.691	51.005	2.388	-0.920	-5.9665	0.9856	40
0	6	6	89.803	90.884	92.759	5.803	-1.081	-6.4323	0.9562	41
0	6	7	33.226	33.203	-33.233	-2.098	0.023	0.1218	0.9942	42
0	6	8	4.093	4.343	-3.929	1.852	-0.250	-0.6188	0.9999	43
0	6	9	29.355	28.660	28.662	2.077	0.695	3.2049	0.9947	44
0	6	10	48.655	46.349	46.539	4.866	2.306	9.9964	0.9811	45
0	8	0	59.135	57.304	58.087	4.982	1.832	14.1061	0.9661	46
0	8	1	6.416	6.556	-6.151	-2.272	-0.140	-0.7960	0.9996	47
0	8	2	45.994	45.809	46.041	3.191	0.185	1.3802	0.9852	48
0	8	3	7.810	7.583	-7.251	2.225	0.227	1.3035	0.9997	49
0	8	4	46.205	47.134	47.168	4.788	-0.928	-6.0758	0.9883	50
0	8	5	11.746	11.305	-11.110	-2.107	0.442	2.4476	0.9994	53
0	8	6	31.789	31.950	31.895	2.964	-0.160	-0.8895	0.9948	54
0	8	7	8.567	8.920	-8.693	2.009	-0.353	-1.4410	0.9996	55
0	8	8	30.929	30.798	30.582	4.246	0.130	0.6022	0.9950	56
0	8	9	8.646	8.315	-8.129	-1.754	0.331	1.2024	0.9996	57
0	10	0	58.117	56.370	57.058	4.176	1.748	11.6362	0.9708	58
0	10	1	52.223	51.273	51.698	2.899	0.949	6.4613	0.9806	59
0	10	2	17.261	16.708	16.321	3.643	0.553	3.5437	0.9983	60
0	10	3	36.925	37.222	-37.258	-2.729	-0.297	-1.9036	0.9927	61
0	10	4	48.278	48.955	49.078	4.025	-0.677	-4.1275	0.9883	62
0	10	5	43.106	43.623	43.729	2.803	-0.517	-2.9160	0.9911	63
0	10	6	20.214	15.912	15.557	3.385	4.302	22.7361	0.9988	64
0	10	7	20.438	20.496	-20.382	-2.358	-0.057	-0.2773	0.9979	65
0	10	8	34.583	35.224	35.158	3.596	-0.641	-2.9938	0.9934	66
0	10	9	28.381	28.501	28.463	2.455	-0.120	-0.5307	0.9953	67

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
0	12	0	59.444	57.484	58.320	3.343	1.960	11.5373	0.9684	68	
0	12	1	53.962	52.653	-53.098	-2.752	1.310	7.8471	0.9806	69	
0	12	2	43.913	43.480	43.513	4.344	0.433	2.5528	0.9886	70	
0	12	3	50.849	51.289	51.556	2.821	-0.440	-2.5483	0.9867	71	
0	12	4	44.980	45.667	45.784	3.196	-0.687	-3.8065	0.9901	72	
0	12	5	37.951	38.255	-38.305	-2.524	-0.304	-1.5946	0.9931	73	
0	12	6	27.554	27.999	27.771	3.569	-0.444	-2.1144	0.9961	74	
0	12	7	36.982	37.413	37.463	2.598	-0.430	-2.0146	0.9925	75	
0	12	8	26.083	26.029	25.927	2.803	0.054	0.2439	0.9962	76	
0	14	0	39.750	38.355	38.305	4.911	1.395	7.0527	0.9864	77	
0	14	1	6.380	6.262	-6.011	1.758	0.118	0.4295	0.9997	78	
0	14	2	22.406	22.417	22.337	2.265	-0.011	-0.0551	0.9969	79	
0	14	3	3.324	2.148	-1.341	-1.678	1.175	2.6888	1.0000	80	
0	14	4	33.944	34.265	34.043	4.715	-0.321	-1.6107	0.9940	81	
0	14	5	9.548	10.105	-9.966	1.686	-0.557	-2.2243	0.9995	82	
0	14	6	18.723	18.567	18.463	2.111	0.156	0.7016	0.9982	83	
0	14	7	5.367	4.603	-4.373	-1.440	0.763	1.6534	0.9999	84	
0	16	0	12.755	12.152	-12.109	1.124	0.603	2.0487	0.9986	85	
0	16	1	16.995	16.314	-16.266	-1.482	0.681	3.0708	0.9976	86	
0	16	2	50.165	49.448	49.605	5.516	0.717	3.4653	0.9815	87	
0	16	4	8.285	8.370	-8.299	1.103	-0.085	-0.2802	0.9996	89	
0	16	5	10.031	10.015	-9.936	-1.274	0.016	0.0630	0.9994	90	
0	18	0	47.035	46.481	46.682	5.295	0.554	2.4464	0.9788	91	
0	18	1	19.441	19.677	19.682	1.098	-0.236	-0.9940	0.9964	92	
0	18	2	12.942	13.314	13.276	1.133	-0.372	-1.4769	0.9984	93	
1	18	2	3.558	3.365	3.366	-0.014	0.193	0.3868	0.9999	94	
1	18	1	5.058	4.903	-4.902	0.128	0.155	0.3692	0.9998	95	
1	18	0	1.951 *	3.826	3.826	0.077	-1.875	-1.2804	0.9999	96	* **
1	17	0	22.273	22.244	22.171	2.337	0.029	0.1299	0.9956	97	
1	17	1	12.947	12.412	12.269	1.933	0.535	2.1913	0.9987	98	
1	17	2	26.510	26.684	26.433	4.159	-0.174	-0.7947	0.9944	99	
1	17	3	12.466	12.157	-12.029	-1.802	0.309	1.2361	0.9990	102	
1	16	5	1.489 *	2.067	2.067	0.011	-0.579	-0.5174	1.0000	103	* **
1	16	4	1.438 *	1.542	1.539	0.098	-0.104	-0.0963	1.0000	104	* **
1	16	3	7.183	7.128	7.129	0.065	0.055	0.1868	0.9997	105	
1	16	2	7.198	7.101	7.103	-0.031	0.097	0.3420	0.9996	106	
1	16	1	2.709	1.827	-1.827	-0.025	0.882	1.5392	1.0000	107	
1	16	0	2.332 *	3.498	3.497	0.113	-1.167	-0.6664	0.9999	108	* **
1	15	0	57.879	57.191	57.726	5.519	0.689	3.5085	0.9726	109	
1	15	1	8.743	8.349	-8.213	-1.513	0.393	1.5638	0.9994	110	
1	15	2	3.853	3.828	3.538	1.462	0.025	0.0612	0.9999	111	
1	15	3	9.074	9.061	8.926	1.571	0.013	0.0508	0.9995	112	
1	15	4	49.093	50.109	50.175	5.290	-1.016	-4.9220	0.9864	113	
1	15	5	5.499	6.223	-6.081	-1.325	-0.723	-2.0200	0.9998	114	
1	15	6	4.007	3.576	3.306	1.363	0.431	0.9745	0.9999	115	
1	14	6	2.928	2.504	2.494	0.216	0.425	0.7776	1.0000	116	
1	14	5	2.766	2.655	2.651	0.140	0.111	0.2129	1.0000	117	
1	14	4	13.957	13.820	-13.824	-0.282	0.136	0.6290	0.9990	118	
1	14	3	1.282 *	0.397	-0.380	-0.116	0.885	0.9198	1.0000	119	* **
1	14	2	1.351 *	1.651	-1.638	0.203	-0.300	-0.2958	1.0000	120	* **
1	14	1	3.666	2.123	2.119	0.135	1.543	3.9623	1.0000	121	
1	14	0	19.879	19.113	-19.140	-0.313	0.766	2.7063	0.9969	122	
1	13	0	6.518	5.652	5.501	1.300	0.866	2.9699	0.9997	123	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
1	13	1	28.794	28.269	28.314	1.411	0.525	2.9249	0.9944	124	
1	13	2	59.514	58.949	59.251	6.003	0.565	3.1519	0.9798	125	
1	13	3	24.088	24.328	-24.331	-1.294	-0.240	-1.2748	0.9970	126	
1	13	4	5.616	5.601	5.458	1.263	0.014	0.0503	0.9998	127	
1	13	5	22.791	23.308	23.296	1.401	-0.517	-2.5737	0.9974	128	
1	13	6	44.923	45.565	45.471	5.521	-0.642	-3.1049	0.9895	129	
1	13	7	16.421	15.840	-15.815	-1.080	0.581	2.4779	0.9986	130	
1	12	8	2.814	2.462	-2.461	0.045	0.352	0.6150	1.0000	131	
1	12	7	9.933	10.148	-10.150	0.050	-0.215	-0.8411	0.9994	132	
1	12	6	5.995	5.320	5.321	-0.025	0.674	2.2307	0.9999	133	
1	12	5	6.572	6.077	-6.076	-0.137	0.495	1.8600	0.9998	134	
1	12	4	2.561	2.134	-2.133	0.063	0.427	0.9113	1.0000	135	
1	12	3	7.852	8.257	-8.258	0.073	-0.404	-1.8022	0.9997	136	
1	12	2	8.552	9.171	9.173	-0.019	-0.618	-2.8207	0.9995	137	
1	12	1	3.251	0.300	-0.277	-0.114	2.952	8.1386	1.0000	138	
1	12	0	3.186	1.728	-1.726	0.071	1.458	1.8549	1.0000	139	
1	11	0	60.850	59.499	60.099	6.253	1.351	8.6121	0.9696	140	
1	11	1	2.256	0.437	-0.334	-0.281	1.819	3.9045	1.0000	141	
1	11	2	23.599	23.800	23.793	1.482	-0.200	-1.2089	0.9967	142	
1	11	3	1.200 *	0.514	-0.511	0.339	0.587	0.6512	1.0000	143	* **
1	11	4	48.370	49.658	49.588	5.995	-1.289	-7.4708	0.9884	144	
1	11	5	1.320 *	0.761	-0.734	-0.199	0.559	0.5643	1.0000	145	* **
1	11	6	17.010	17.421	17.378	1.393	-0.411	-1.9527	0.9985	146	
1	11	7	1.446 *	0.533	-0.389	0.364	0.913	0.8413	1.0000	147	* **
1	11	8	34.708	34.897	34.612	5.280	-0.189	-0.8682	0.9934	148	
1	10	8	3.187	2.747	-2.745	-0.109	0.440	0.8573	1.0000	151	
1	10	7	3.240	2.948	2.945	0.119	0.292	0.6446	1.0000	152	
1	10	6	5.973	5.766	5.764	0.144	0.208	0.7263	0.9998	153	
1	10	5	10.590	10.775	10.778	-0.023	-0.185	-0.9064	0.9995	154	
1	10	4	3.237	2.984	2.983	-0.092	0.252	0.7207	1.0000	155	
1	10	3	1.138 *	0.822	0.815	0.104	0.316	0.3702	1.0000	156	* **
1	10	2	13.821	14.205	14.212	0.186	-0.384	-2.3326	0.9988	157	
1	10	1	7.513	7.608	7.609	-0.062	-0.095	-0.5023	0.9996	158	
1	10	0	4.545	7.249	7.250	-0.082	-2.704	-5.4981	0.9995	159	
1	9	0	3.806	3.836	3.656	1.161	-0.030	-0.1150	0.9999	160	
1	9	1	24.811	24.781	-24.828	-0.712	0.030	0.2147	0.9954	161	
1	9	2	98.236	98.409	101.223	6.858	-0.173	-1.2198	0.9409	162	
1	9	3	23.144	23.358	23.380	0.760	-0.215	-1.4005	0.9971	163	
1	9	4	2.530	2.463	2.191	1.126	0.067	0.1497	1.0000	164	
1	9	5	16.929	17.165	-17.166	-0.606	-0.236	-1.3194	0.9986	165	
1	9	6	65.355	66.165	66.586	6.295	-0.810	-4.4434	0.9786	166	
1	9	7	14.547	15.201	15.192	0.738	-0.654	-2.9453	0.9988	167	
1	9	8	2.935	2.063	1.790	1.026	0.871	1.7195	1.0000	168	
1	9	9	9.305	9.155	-9.145	-0.466	0.150	0.5535	0.9995	169	
1	8	9	6.542	6.691	6.691	0.099	-0.149	-0.4707	0.9997	170	
1	8	8	4.111	3.625	3.617	0.248	0.485	1.1886	0.9999	171	
1	8	7	1.379 *	1.657	-1.656	-0.042	-0.278	-0.2684	1.0000	172	* **
1	8	6	10.023	10.046	-10.044	-0.286	-0.023	-0.1103	0.9995	173	
1	8	5	10.092	10.138	10.140	0.107	-0.046	-0.2422	0.9995	174	
1	8	4	3.440	3.182	-3.173	0.237	0.258	0.8250	0.9999	175	
1	8	3	5.576	5.054	-5.054	-0.064	0.523	2.5686	0.9999	176	
1	8	2	24.867	25.297	-25.350	-0.349	-0.430	-3.1369	0.9957	177	
1	8	1	11.184	11.323	11.329	0.092	-0.139	-0.9300	0.9990	178	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
1	8	0	12.358	12.033	-12.040	0.228	0.325	2.1423	0.9986	179	
1	7	0	118.409	115.737	124.395	6.845	2.672	16.8860	0.8630	180	
1	7	1	2.763	2.589	2.355	1.076	0.174	0.5770	0.9999	181	
1	7	2	2.661	1.672	0.807	1.464	0.989	3.0408	1.0000	182	
1	7	3	2.100	1.547	1.184	-0.995	0.554	1.3420	1.0000	183	
1	7	4	90.789	92.553	94.523	6.564	-1.764	-12.1149	0.9541	184	
1	7	5	3.025	2.238	1.972	1.057	0.788	2.0786	1.0000	185	
1	7	6	6.560	2.111	1.599	1.378	4.449	19.0551	1.0000	186	
1	7	7	1.384 *	2.238	2.075	-0.838	-0.854	-0.8219	1.0000	187	* **
1	7	8	55.258	55.353	55.504	5.787	-0.095	-0.4724	0.9839	188	
1	7	9	1.490 *	2.395	2.202	0.942	-0.904	-0.8078	1.0000	189	* **
1	6	10	1.572 *	3.178	-3.178	0.047	-1.606	-1.3603	0.9999	190	* **
1	6	9	6.885	6.873	-6.874	-0.022	0.012	0.0379	0.9997	191	
1	6	8	4.691	4.290	4.290	-0.046	0.401	1.0786	0.9999	192	
1	6	7	13.912	13.844	-13.850	-0.068	0.069	0.3310	0.9990	193	
1	6	6	3.227	4.338	-4.338	0.063	-1.111	-2.8149	0.9999	194	
1	6	5	8.001	8.556	-8.557	-0.026	-0.554	-2.8214	0.9996	195	
1	6	4	8.957	9.501	9.503	-0.046	-0.543	-3.1585	0.9995	196	
1	6	3	15.832	16.190	-16.204	-0.055	-0.358	-2.6052	0.9983	197	
1	6	2	5.203	5.763	-5.763	0.074	-0.560	-3.0196	0.9997	200	
1	6	1	2.341	1.443	-1.443	0.009	0.898	3.0696	1.0000	201	
1	6	0	15.980	15.379	15.401	-0.046	0.601	4.8910	0.9971	202	
1	5	0	60.991	59.886	61.394	2.548	1.106	10.3915	0.9498	203	
1	5	1	41.854	42.037	-42.401	-2.001	-0.184	-1.7170	0.9807	204	
1	5	2	78.854	81.397	83.485	5.922	-2.543	-22.3146	0.9458	205	
1	5	3	31.545	32.527	32.589	1.983	-0.982	-7.8197	0.9925	206	
1	5	4	45.162	46.368	46.621	2.458	-1.206	-8.7254	0.9864	207	
1	5	5	26.215	26.641	-26.635	-1.840	-0.427	-2.7052	0.9957	208	
1	5	6	46.535	47.105	47.081	5.447	-0.570	-3.3507	0.9878	209	
1	5	8	27.312	26.881	26.846	2.205	0.431	2.1149	0.9959	211	
1	5	9	15.673	14.467	-14.396	-1.539	1.206	5.2136	0.9985	212	
1	5	10	30.215	28.549	28.283	4.607	1.667	7.1632	0.9926	213	
1	4	10	7.057	7.372	-7.374	-0.057	-0.315	-0.9251	0.9995	214	
1	4	9	7.175	6.143	6.140	0.228	1.032	3.4403	0.9997	215	
1	4	8	5.504	5.607	5.607	0.050	-0.103	-0.3123	0.9998	216	
1	4	7	5.547	5.730	5.728	-0.143	-0.183	-0.6160	0.9998	217	
1	4	6	3.394	2.706	-2.706	-0.029	0.688	1.9411	1.0000	218	
1	4	5	10.113	10.271	10.271	0.252	-0.157	-0.8879	0.9993	219	
1	4	4	22.975	24.382	24.433	0.100	-1.407	-9.8853	0.9958	220	
1	4	3	9.349	8.655	8.656	-0.186	0.694	4.8314	0.9994	221	
1	4	2	4.450	4.709	4.709	0.001	-0.259	-1.5667	0.9998	222	
1	4	1	1.518	1.897	1.882	0.232	-0.378	-1.1353	1.0000	223	
1	4	0	60.309	56.740	58.298	0.123	3.569	36.2213	0.9473	224	
1	3	0	120.743	117.838	135.368	5.724	2.906	14.4788	0.7564	225	
1	3	1	84.722	86.099	90.855	2.917	-1.377	-9.9523	0.8971	226	
1	3	2	53.067	53.711	54.440	2.952	-0.644	-6.1323	0.9705	227	
1	3	3	70.847	72.846	-74.526	-2.829	-1.999	-16.8148	0.9541	228	
1	3	4	85.307	88.331	90.967	5.488	-3.024	-22.3821	0.9395	229	
1	3	5	55.564	56.607	57.164	2.748	-1.043	-6.9423	0.9783	230	
1	3	6	27.149	27.422	27.351	2.728	-0.273	-1.6051	0.9953	231	
1	3	7	40.211	39.966	-40.088	-2.508	0.244	1.3336	0.9901	232	
1	3	8	46.781	45.890	45.993	4.837	0.891	4.4244	0.9846	233	
1	3	9	31.217	29.368	29.385	2.367	1.849	8.3227	0.9924	234	

CYCLE THREE. STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIG A	EXT. FACTOR		
1	3	10	16.257		14.591	14.822	2.334	1.266	5.0117	0.9981	235	
1	2	10	1.546	*	0.520	0.504	0.128	1.026	0.8839	1.0000	236	* **
1	2	9	1.487	*	0.776	-0.761	-0.153	0.711	0.6367	1.0000	237	* **
1	2	8	2.594		1.806	1.802	-0.120	0.788	1.2907	1.0000	238	
1	2	7	13.265		13.112	13.118	0.258	0.153	0.7420	0.9987	239	
1	2	6	7.444		7.940	-7.941	0.105	-0.496	-2.3485	0.9996	240	
1	2	5	3.281		2.954	-2.947	-0.192	0.327	0.9742	0.9999	241	
1	2	4	8.344		9.222	-9.224	-0.182	-0.878	-5.1689	0.9993	242	
1	2	3	22.870		23.075	23.139	0.266	-0.206	-1.6747	0.9944	243	
1	2	2	48.745		48.021	-48.698	0.078	0.724	7.0451	0.9724	244	
1	2	1	16.259		15.879	-15.909	-0.236	0.380	4.1250	0.9961	245	
1	2	0	26.101		25.033	-25.228	-0.210	1.069	12.5806	0.9845	246	
1	1	1	52.341		53.615	-54.979	-2.727	-1.275	-11.1694	0.9487	250	
1	1	3	45.995		48.027	48.601	2.680	-2.032	-16.8598	0.9736	252	
1	1	4	32.011		33.507	33.502	3.504	-1.496	-10.5574	0.9895	253	
1	1	5	28.777		29.211	-29.205	-2.533	-0.433	-2.8073	0.9929	254	
1	1	6	68.463		68.037	69.243	4.650	0.426	2.5369	0.9611	255	
1	1	7	24.322		23.390	23.326	2.402	0.933	4.7997	0.9950	256	
1	1	8	18.371		17.670	17.417	3.114	0.701	3.2255	0.9973	257	
1	1	9	14.860		14.384	-14.234	-2.151	0.476	1.9683	0.9984	258	
1	1	10	39.533		37.042	37.025	3.951	2.491	11.0174	0.9857	259	
1	0	9	14.804		13.619	-13.628	-0.027	1.186	4.9698	0.9986	260	
1	0	7	6.773		6.335	-6.336	-0.069	0.438	1.6380	0.9996	261	
1	0	5	24.408		24.770	-24.853	-0.030	-0.363	-2.2135	0.9933	262	
1	0	3	8.895		7.756	-7.759	-0.056	1.139	7.7104	0.9992	263	
1	0	1	24.047		24.739	-24.940	0.008	-0.692	-7.0006	0.9839	264	
2	0	0	88.536		88.163	97.120	7.269	0.373	2.3893	0.8195	265	
2	0	2	3.260		1.388	-0.660	1.221	1.872	6.8352	1.0000	266	
2	0	4	83.448		84.705	87.619	6.988	-1.257	-8.3770	0.9287	267	
2	0	6	6.532		6.423	6.313	1.189	0.110	0.4000	0.9996	268	
2	0	8	57.740		54.509	54.754	6.197	3.231	15.8142	0.9785	269	
2	0	10	12.456		11.775	11.730	1.096	0.681	2.6360	0.9991	270	
2	1	9	13.170		12.296	12.301	0.204	0.873	3.5873	0.9989	272	
2	1	8	9.954		9.575	9.569	0.425	0.379	1.5219	0.9993	273	
2	1	7	12.812		12.413	-12.420	-0.139	0.400	1.8314	0.9987	274	
2	1	6	12.186		11.791	-11.789	-0.450	0.395	1.9666	0.9989	275	
2	1	5	22.057		22.813	22.858	0.218	-0.756	-4.4983	0.9960	276	
2	1	4	21.146		21.975	22.013	0.499	-0.829	-5.4021	0.9960	277	
2	1	3	23.058		23.931	-23.995	-0.176	-0.873	-6.3832	0.9946	278	
2	1	2	12.898		13.596	-13.602	-0.480	-0.698	-5.4520	0.9979	279	
2	1	1	34.158		34.414	34.640	0.207	-0.256	-2.4018	0.9870	280	
2	1	0	37.112		35.325	35.674	0.528	1.788	18.1357	0.9803	281	
2	2	0	25.116		24.670	24.731	1.638	0.445	4.2072	0.9907	282	
2	2	1	13.105		12.101	12.089	0.707	1.005	9.0222	0.9985	283	
2	2	3	9.508		8.976	8.957	-0.629	0.532	3.3815	0.9993	285	
2	2	4	16.493		16.011	15.948	1.577	0.482	3.0961	0.9981	286	
2	2	5	14.189		13.948	13.939	0.712	0.241	1.3917	0.9987	287	
2	2	6	78.624		79.136	80.512	6.376	-0.512	-2.9587	0.9601	288	
2	2	7	10.115		9.549	9.538	-0.524	0.566	2.3638	0.9993	289	
2	2	8	9.328		6.522	6.368	1.411	2.807	10.9821	0.9997	290	
2	2	9	11.444		9.184	9.166	0.625	2.260	8.7689	0.9994	291	
2	2	10	44.932		42.647	42.593	5.363	2.285	9.9219	0.9869	292	
2	3	10	5.883		5.557	-5.557	0.030	0.326	0.8463	0.9998	293	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
2	3	9	1.543 *	2.633	-2.631	0.100	-1.090	-0.9407	0.9999	294	* **
2	3	8	9.035	8.287	8.289	-0.029	0.748	2.7415	0.9995	295	
2	3	7	3.807	3.257	-3.256	-0.088	0.550	1.4279	0.9999	298	
2	3	6	11.082	11.291	-11.295	0.041	-0.208	-1.0352	0.9992	299	
2	3	5	3.394	4.330	-4.329	0.104	-0.936	-2.6268	0.9999	300	
2	3	4	15.089	15.087	15.099	-0.035	0.001	0.0093	0.9984	301	
2	3	3	4.102	4.514	-4.513	-0.107	-0.411	-1.6204	0.9998	302	
2	3	2	15.668	16.001	-16.018	0.048	-0.333	-2.6768	0.9979	303	
2	3	1	0.873 *	1.117	-1.112	0.109	-0.244	-0.3729	1.0000	304	* **
2	3	0	19.349	19.038	19.086	-0.038	0.311	2.8328	0.9949	305	
2	4	0	126.134	123.732	136.162	6.480	2.402	9.9260	0.8239	306	
2	4	1	55.407	54.399	-55.173	-1.810	1.009	8.9904	0.9711	307	
2	4	2	44.594	45.215	45.521	2.086	-0.621	-5.2044	0.9845	308	
2	4	3	33.070	32.935	33.010	1.756	0.135	1.0244	0.9927	309	
2	4	4	87.349	89.167	91.255	6.201	-1.818	-12.5647	0.9504	310	
2	4	5	42.126	42.344	-42.536	-1.698	-0.218	-1.3552	0.9894	311	
2	4	6	23.297	23.394	23.350	1.924	-0.097	-0.5384	0.9970	312	
2	4	7	16.395	15.435	15.365	1.573	0.959	4.6838	0.9987	313	
2	4	8	49.025	46.320	46.318	5.440	2.705	13.1871	0.9865	314	
2	4	9	24.984	23.924	-23.933	-1.430	1.061	4.5587	0.9956	315	
2	4	10	10.739	10.241	10.112	1.648	0.498	1.7644	0.9992	316	
2	5	10	1.528 *	0.784	-0.756	-0.207	0.745	0.6488	1.0000	317	* **
2	5	9	10.649	10.684	-10.681	-0.384	-0.035	-0.1266	0.9992	318	
2	5	8	3.007	2.403	2.390	0.245	0.604	1.1903	1.0000	319	
2	5	7	18.252	18.040	18.049	0.494	0.212	1.0373	0.9983	320	
2	5	6	4.886	4.853	-4.846	-0.263	0.033	0.1097	0.9999	321	
2	5	5	20.152	20.380	-20.398	-0.464	-0.228	-1.3650	0.9976	322	
2	5	4	1.115 *	0.646	0.590	0.265	0.469	0.5599	1.0000	323	* **
2	5	3	28.690	29.504	29.580	0.530	-0.814	-6.0318	0.9945	324	
2	5	2	11.424	11.499	-11.501	-0.299	-0.075	-0.5373	0.9991	325	
2	5	1	31.221	31.348	-31.484	-0.518	-0.127	-1.0684	0.9911	326	
2	5	0	4.200	3.480	-3.470	0.271	0.720	3.0301	0.9999	327	
2	6	0	11.167	11.503	11.283	2.279	-0.336	-2.3491	0.9986	328	
2	6	1	33.073	32.344	32.405	2.286	0.729	5.8186	0.9913	329	
2	6	2	68.460	68.221	69.051	5.856	0.239	1.8441	0.9691	330	
2	6	3	30.124	30.153	-30.154	-2.200	-0.029	-0.2088	0.9947	331	
2	6	5	22.701	22.167	22.089	2.171	0.534	3.1741	0.9974	333	
2	6	6	51.532	51.605	51.678	5.421	-0.073	-0.4101	0.9863	334	
2	6	7	18.791	18.224	-18.137	-1.930	0.567	2.8045	0.9983	335	
2	6	8	15.314	15.505	15.382	2.028	-0.191	-0.8448	0.9987	336	
2	6	9	12.727	12.086	11.943	1.887	0.642	2.5721	0.9999	337	
2	7	9	1.474 *	2.496	-2.492	0.149	-1.023	-0.9240	1.0000	338	* **
2	7	8	10.618	11.696	-11.695	-0.329	-1.078	-4.2128	0.9993	339	
2	7	7	9.277	8.549	8.550	-0.079	0.728	3.0541	0.9996	340	
2	7	6	17.040	16.779	16.786	0.375	0.262	1.3696	0.9986	341	
2	7	5	5.564	5.526	-5.524	0.158	0.039	0.1563	0.9998	342	
2	7	4	16.287	17.465	-17.475	-0.364	-1.178	-7.2011	0.9984	343	
2	7	3	12.125	12.158	12.163	-0.113	-0.033	-0.2127	0.9992	344	
2	7	2	28.257	28.392	28.463	0.418	-0.135	-0.9828	0.9948	347	
2	7	1	10.140	10.385	-10.389	0.144	-0.245	-1.5812	0.9992	348	
2	7	0	20.857	20.377	-20.414	-0.375	0.480	3.4531	0.9960	349	
2	8	0	82.337	80.548	82.766	4.995	1.789	12.8959	0.9437	350	
2	8	1	34.122	33.689	-33.742	-2.405	0.433	3.1015	0.9918	351	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
3	11	1	4.846	3.729	-3.716	-0.312	1.117	3.7427	0.9999	464	
3	11	2	16.992	16.839	16.800	1.314	0.153	0.8237	0.9985	465	
3	11	3	7.513	7.896	7.888	0.397	-0.384	-1.5257	0.9997	466	
3	11	4	47.093	49.007	48.921	5.904	-1.915	-10.2730	0.9891	467	
3	11	5	1.399 *	0.513	0.469	-0.207	0.886	0.8436	1.0000	468	* **
3	11	6	12.727	12.712	12.658	1.231	0.015	0.0624	0.9992	469	
3	11	7	7.938	7.944	7.934	0.428	-0.006	-0.0211	0.9997	470	
3	10	8	3.591	3.554	3.545	-0.261	0.037	0.0749	0.9999	471	
3	10	7	12.246	12.927	12.929	0.312	-0.682	-2.8135	0.9991	472	
3	10	6	5.679	6.394	-6.387	0.300	-0.715	-2.2396	0.9998	473	
3	10	5	26.181	27.323	-27.368	-0.335	-1.142	-5.9179	0.9966	474	
3	10	4	2.463	0.403	0.228	-0.332	2.060	4.0185	1.0000	475	
3	10	3	21.943	22.392	22.415	0.340	-0.449	-2.5434	0.9977	476	
3	10	2	13.841	13.300	-13.302	0.305	0.541	2.9530	0.9991	477	
3	10	1	31.166	30.361	-30.448	-0.354	0.805	4.8258	0.9542	478	
3	10	0	2.420	2.354	-2.327	-0.361	0.065	0.1368	1.0000	479	
3	9	0	4.730	4.276	-4.094	1.237	0.454	1.6297	0.9999	480	
3	9	1	10.719	10.987	-10.980	-0.498	-0.268	-1.4473	0.9992	481	
3	9	2	72.494	73.622	74.393	6.417	-1.128	-7.1324	0.9721	482	
3	9	3	9.285	9.424	9.411	0.541	-0.139	-0.6639	0.9996	483	
3	9	4	2.441	1.804	-1.338	1.210	0.637	1.2855	1.0000	484	
3	9	5	7.792	8.567	-8.558	-0.413	-0.775	-3.1719	0.9997	485	
3	9	6	54.148	55.330	55.431	5.912	-1.183	-6.0595	0.9852	486	
3	9	7	6.489	6.243	6.220	0.535	0.246	0.8218	0.9998	487	
3	9	8	2.798	2.646	2.395	1.124	0.152	0.2570	1.0000	488	
3	8	8	17.721	17.395	17.395	0.693	0.326	1.4424	0.9984	489	
3	8	7	1.384 *	0.128	-0.090	-0.091	1.256	1.2090	1.0000	490	* **
3	8	6	18.200	18.491	-18.494	-0.701	-0.291	-1.4361	0.9983	491	
3	8	5	5.347	5.340	-5.339	0.132	0.007	0.0240	0.9999	494	
3	8	4	35.172	35.582	35.678	0.828	-0.410	-2.4412	0.9941	495	
3	8	3	1.147 *	1.172	1.166	-0.119	-0.026	-0.0299	1.0000	496	* **
3	8	2	20.232	20.241	-20.250	-0.734	-0.009	-0.0594	0.9978	497	
3	8	1	5.287	4.614	-4.613	0.130	0.673	2.9560	0.9999	498	
3	8	0	48.185	47.739	48.161	0.882	0.446	2.9745	0.9822	499	
3	7	0	92.800	90.321	93.191	6.430	2.479	17.3686	0.9349	500	
3	7	1	14.567	14.812	14.774	1.204	-0.245	-1.5810	0.9985	501	
3	7	2	19.164	19.410	19.362	1.637	-0.246	-1.6166	0.9979	502	
3	7	3	16.091	16.448	-16.419	-1.147	-0.357	-2.1895	0.9986	503	
3	7	4	70.230	71.877	72.513	6.159	-1.647	-10.2111	0.9755	504	
3	7	5	8.150	8.230	8.150	1.156	-0.080	-0.3549	0.9997	505	
3	7	6	11.899	11.984	11.892	1.521	-0.085	-0.3855	0.9993	506	
3	7	7	11.537	11.618	-11.580	-0.989	-0.081	-0.3489	0.9993	507	
3	7	8	43.352	44.020	43.915	5.414	-0.667	-3.0978	0.9897	508	
3	7	9	5.311	5.036	4.931	1.023	0.275	0.7263	0.9998	509	
3	6	9	17.510	17.214	17.230	0.121	0.296	1.2642	0.9981	510	
3	6	8	1.454 *	0.539	-0.487	-0.233	0.914	0.8381	1.0000	511	* **
3	6	7	4.253	3.949	-3.949	0.064	0.305	0.7930	0.9999	512	
3	6	6	1.382 *	0.664	-0.608	0.266	0.718	0.6924	1.0000	513	* **
3	6	5	26.740	26.907	26.956	0.105	-0.167	-0.9523	0.9964	514	
3	6	3	12.641	12.823	-12.828	0.025	-0.182	-1.0866	0.9991	516	
3	6	2	1.097 *	1.646	-1.621	0.288	-0.549	-0.6673	1.0000	517	* **
3	6	1	27.051	26.932	27.001	0.046	0.118	0.8490	0.9949	518	
3	6	0	3.804	3.399	-3.386	-0.291	0.405	1.2009	0.9999	519	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	5	0	38.865	38.474	38.669	2.296	0.391	2.9570	0.9865	520
3	5	1	22.558	22.866	-22.832	-1.889	-0.308	-2.2770	0.9961	521
3	5	2	79.441	80.336	81.677	5.902	-0.895	-6.6122	0.9624	522
3	5	3	25.789	26.236	26.216	1.904	-0.446	-3.0413	0.9963	523
3	5	4	28.435	28.990	28.970	2.210	-0.555	-3.4902	0.9956	524
3	5	5	11.826	11.981	-11.863	-1.712	-0.155	-0.8064	0.9992	525
3	5	6	50.321	50.969	51.019	5.420	-0.649	-3.5280	0.9869	526
3	5	7	18.300	18.005	17.936	1.743	0.295	1.4168	0.9983	527
3	5	8	16.846	17.047	16.946	1.975	-0.201	-0.8862	0.9984	528
3	5	9	6.034	5.959	-5.787	-1.428	0.075	0.2212	0.9998	529
3	4	9	10.259	10.094	10.082	0.562	0.165	0.5869	0.9993	530
3	4	8	13.811	14.336	-14.345	0.005	-0.525	-2.1894	0.9987	531
3	4	7	24.005	24.105	-24.135	-0.588	-0.100	-0.4855	0.9969	532
3	4	6	15.923	15.558	15.567	-0.013	0.366	1.8188	0.9987	533
3	4	5	18.836	19.298	19.307	0.636	-0.462	-2.5791	0.9980	534
3	4	4	31.759	32.826	-32.927	-0.028	-1.068	-6.7782	0.9939	535
3	4	3	35.569	36.644	-36.779	-0.666	-1.075	-7.5465	0.9923	536
3	4	2	15.806	16.018	16.031	-0.045	-0.213	-1.5006	0.9984	537
3	4	1	34.563	34.204	34.354	0.678	0.359	2.8134	0.9909	538
3	4	0	50.971	49.879	-50.481	-0.044	1.092	8.6596	0.9763	539
3	3	0	81.887	80.884	83.426	5.412	1.003	8.2126	0.9360	540
3	3	1	59.938	59.707	60.468	2.553	0.231	1.8813	0.9733	543
3	3	2	24.905	25.520	25.413	2.864	-0.616	-4.5858	0.9958	544
3	3	3	50.458	51.184	-51.548	-2.477	-0.726	-5.0331	0.9837	545
3	3	4	64.223	64.667	65.294	5.202	-0.444	-2.8548	0.9747	546
3	3	5	38.900	39.246	39.345	2.404	-0.347	-2.0381	0.9913	547
3	3	6	19.765	20.280	20.126	2.671	-0.514	-2.6223	0.9977	548
3	3	7	29.372	29.763	-29.759	-2.193	-0.391	-1.9208	0.9949	549
3	3	8	41.789	41.181	41.154	4.612	0.608	2.6222	0.9889	550
3	3	9	23.587	22.498	22.444	2.069	1.089	4.6523	0.9963	551
3	2	10	13.968	13.321	13.324	0.388	0.647	2.5030	0.9988	552
3	2	9	10.095	9.695	-9.687	-0.461	0.400	1.3972	0.9993	553
3	2	8	21.367	20.686	-20.715	-0.437	0.680	3.0183	0.9968	554
3	2	7	4.952	4.912	4.882	0.544	0.040	0.1091	0.9998	555
3	2	6	32.291	32.067	32.161	0.500	0.225	1.2097	0.9939	556
3	2	5	16.710	16.858	-16.864	-0.560	-0.148	-0.8171	0.9983	557
3	2	4	25.511	26.785	-26.843	-0.458	-1.274	-7.8909	0.9954	558
3	2	3	10.807	10.622	10.609	0.595	0.185	1.1203	0.9992	559
3	2	2	61.737	63.066	63.946	0.576	-1.329	-10.0984	0.9726	560
3	2	1	19.005	18.945	-18.960	-0.605	0.060	0.4797	0.9974	561
3	2	0	29.065	28.261	-28.376	-0.461	0.804	6.6846	0.9916	562
3	1	0	68.679	66.868	68.395	3.766	1.811	15.5021	0.9530	563
3	1	1	45.412	46.559	-46.867	-2.688	-1.147	-9.2061	0.9837	564
3	1	2	74.922	77.983	79.810	4.660	-3.061	-22.4955	0.9515	565
3	1	3	32.459	33.495	33.535	2.613	-1.036	-6.8973	0.9916	566
3	1	4	46.462	47.475	47.713	3.613	-1.012	-6.3798	0.9844	567
3	1	5	33.234	34.072	-34.110	-2.521	-0.838	-4.8072	0.9923	568
3	1	6	46.376	46.471	46.625	4.286	-0.095	-0.5120	0.9851	569
3	1	7	18.091	17.342	17.205	2.328	0.749	3.4479	0.9977	570
3	1	8	28.406	25.862	25.725	3.195	2.545	11.7688	0.9953	571
3	1	9	20.583	19.569	-19.477	-2.147	1.014	4.1877	0.9974	572
3	1	10	27.678	26.023	25.827	3.629	1.655	7.0161	0.9956	573
3	0	9	3.161	0.408	-0.340	0.226	2.753	4.5841	1.0000	574

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
3	0	7	23.668	22.405	22.446	-0.048	1.263	5.9650	0.9964	575	
3	0	3	29.865	30.478	30.602	-0.110	-0.613	-3.7061	0.9919	577	
3	0	1	16.345	16.954	-16.978	0.188	-0.609	-4.2244	0.9971	578	
4	0	2	18.799	18.473	18.432	1.532	0.326	1.8877	0.9976	580	
4	0	4	89.916	90.092	92.477	6.453	-0.177	-0.9815	0.9445	581	
4	0	6	8.842	7.871	7.745	1.409	0.971	3.5756	0.9996	582	
4	0	8	54.347	51.840	51.956	5.649	2.507	11.2732	0.9839	583	
4	1	9	1.572 *	1.075	1.065	0.151	0.496	0.4203	1.0000	584	* **
4	1	8	11.876	11.343	11.327	0.693	0.532	1.9992	0.9992	585	
4	1	7	8.547	7.906	-7.907	-0.083	0.641	2.2534	0.9996	586	
4	1	6	17.578	17.420	-17.420	-0.758	0.158	0.7412	0.9981	587	
4	1	5	4.285	4.260	4.258	0.144	0.025	0.0686	0.9999	588	
4	1	4	13.899	14.131	14.118	0.768	-0.232	-1.2052	0.9988	589	
4	1	3	10.742	11.189	-11.193	-0.115	-0.447	-2.2782	0.9992	592	
4	1	2	30.766	31.722	-31.812	-0.849	-0.956	-6.0877	0.9936	593	
4	1	1	7.629	7.836	7.837	0.133	-0.207	-1.1008	0.9996	594	
4	1	0	14.393	14.257	14.247	0.792	0.136	0.9053	0.9984	595	
4	2	0	14.753	14.854	14.786	1.548	-0.100	-0.6808	0.9982	596	
4	2	1	13.149	12.569	12.545	0.861	0.579	3.7889	0.9991	597	
4	2	2	75.401	76.244	77.215	6.481	-0.843	-5.6561	0.9682	598	
4	2	3	19.994	19.782	-19.785	-0.866	0.213	1.2608	0.9977	599	
4	2	4	13.125	13.457	13.380	1.506	-0.332	-1.7147	0.9990	600	
4	2	5	6.970	3.479	3.389	0.788	3.491	13.8110	0.9999	601	
4	2	6	53.054	53.188	53.270	5.969	-0.134	-0.6822	0.9846	602	
4	2	7	15.810	15.143	-15.133	-0.778	0.668	2.8706	0.9986	603	
4	2	8	12.271	11.782	11.706	1.381	0.489	1.9048	0.9991	604	
4	2	9	2.979	0.774	0.371	0.679	2.205	3.7804	1.0000	605	
4	3	9	4.061	4.040	4.032	0.267	0.021	0.0409	0.9999	606	
4	3	8	8.183	7.673	7.672	-0.208	0.510	1.6796	0.9996	607	
4	3	7	7.825	7.999	7.999	-0.105	-0.174	-0.5984	0.9996	608	
4	3	6	10.503	10.871	-10.872	0.237	-0.368	-1.5388	0.9994	609	
4	3	5	4.507	4.493	4.485	0.276	0.014	0.0425	0.9999	610	
4	3	4	13.456	13.094	13.098	-0.244	0.362	1.9301	0.9991	611	
4	3	3	7.733	8.164	8.164	-0.168	-0.430	-2.0600	0.9996	612	
4	3	2	17.206	16.547	-16.557	0.259	0.659	4.3128	0.9986	613	
4	3	1	1.079 *	0.736	-0.697	0.236	0.343	0.4236	1.0000	614	* **
4	3	0	15.875	15.682	15.695	-0.257	0.193	1.2934	0.9981	615	
4	4	0	76.221	74.139	75.467	6.154	2.082	14.4854	0.9588	616	
4	4	1	15.404	15.183	-15.127	-1.426	0.221	1.4415	0.9986	617	
4	4	2	11.129	11.308	11.165	1.817	-0.179	-1.0461	0.9993	618	
4	4	3	20.938	21.132	21.105	1.455	-0.193	-1.1895	0.9978	619	
4	4	4	60.890	61.602	61.921	5.909	-0.712	-4.2062	0.9808	620	
4	4	5	5.784	5.543	-5.394	-1.278	0.240	0.8498	0.9998	621	
4	4	6	11.287	11.091	10.962	1.711	0.195	0.8560	0.9994	622	
4	4	7	16.758	16.596	16.554	1.340	0.162	0.7107	0.9986	623	
4	4	8	41.945	41.665	41.558	5.227	0.280	1.2871	0.9895	624	
4	4	9	1.606 *	2.575	-2.346	-1.062	-0.969	-0.8030	1.0000	625	* **
4	5	9	11.602	11.136	-11.127	-0.549	0.466	1.7534	0.9992	626	
4	5	8	8.437	8.239	8.228	0.461	0.198	0.7015	0.9996	627	
4	5	7	11.589	11.808	11.792	0.689	-0.220	-0.9297	0.9993	628	
4	5	6	6.932	7.833	-7.820	-0.464	-0.901	-3.3194	0.9997	629	
4	5	5	19.654	19.666	-19.673	-0.670	-0.012	-0.0626	0.9981	630	
4	5	4	17.805	18.167	18.173	0.553	-0.362	-2.0231	0.9984	631	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
4	5	3	19.769	20.186	20.192	0.743	-0.418	-2.5221	0.9981	632	
4	5	2	6.769	6.905	-6.888	-0.488	-0.135	-0.6604	0.9998	633	
4	5	1	24.594	24.759	-24.795	-0.739	-0.165	-1.0859	0.9962	634	
4	5	0	25.799	25.653	25.710	0.590	0.146	0.9739	0.9951	635	
4	6	0	34.492	34.036	34.089	2.510	0.456	2.9718	0.9916	636	
4	6	2	77.493	77.337	78.316	5.429	0.155	1.0066	0.9705	638	
4	6	3	28.642	28.130	-28.114	-1.964	0.512	3.1468	0.9963	641	
4	6	4	24.531	25.024	24.945	2.403	-0.492	-2.8049	0.9971	642	
4	6	5	25.828	25.713	25.679	1.963	0.114	0.6069	0.9968	643	
4	6	6	50.205	50.624	50.698	4.966	-0.420	-2.1311	0.9876	644	
4	6	7	18.111	18.046	-17.979	-1.713	0.065	0.2921	0.9984	645	
4	6	8	11.298	11.910	11.725	2.116	-0.612	-2.3181	0.9992	646	
4	7	8	5.890	6.701	-6.688	-0.425	-0.811	-2.4039	0.9998	647	
4	7	7	4.396	4.725	-4.713	-0.332	-0.329	-0.7849	0.9999	648	
4	7	6	8.240	7.851	7.837	0.477	0.389	1.4784	0.9997	649	
4	7	5	2.574	1.933	-1.891	0.402	0.641	1.2408	1.0000	650	
4	7	4	14.957	15.691	-15.691	-0.506	-0.733	-3.8683	0.9989	651	
4	7	3	3.767	4.040	-4.021	-0.395	-0.273	-0.8305	0.9959	652	
4	7	2	8.045	8.426	8.412	0.502	-0.380	-1.8674	0.9997	653	
4	7	1	1.165 *	0.773	0.651	0.416	0.392	0.4486	1.0000	654	* **
4	7	0	21.745	21.155	-21.182	-0.538	0.590	3.5881	0.9968	655	
4	8	0	42.977	42.040	42.050	4.604	0.938	5.7011	0.9877	656	
4	8	1	28.224	27.980	-27.941	-2.404	0.243	1.4628	0.9954	657	
4	8	2	31.213	31.003	30.930	3.001	0.209	1.2580	0.9954	658	
4	8	3	18.630	18.958	18.826	2.365	-0.328	-1.8292	0.9984	659	
4	8	4	35.586	36.172	36.008	4.424	-0.587	-3.2521	0.9941	660	
4	8	5	25.781	25.745	-25.688	-2.226	0.036	0.1867	0.9969	661	
4	8	6	23.853	24.612	24.491	2.786	-0.759	-3.6142	0.9970	662	
4	8	7	9.703	9.841	9.607	2.141	-0.137	-0.5267	0.9995	663	
4	8	8	26.397	26.492	26.250	3.922	-0.095	-0.4258	0.9963	664	
4	9	7	2.961	1.709	1.651	0.444	1.251	2.4042	1.0000	665	
4	9	6	7.372	6.545	6.544	0.138	0.827	2.9644	0.9998	666	
4	9	5	9.370	9.825	9.822	-0.325	-0.455	-1.8568	0.9995	667	
4	9	4	10.231	10.155	-10.157	-0.121	0.076	0.3437	0.9995	668	
4	9	3	3.329	1.695	-1.634	0.453	1.634	4.3934	1.0000	669	
4	9	2	8.525	8.898	8.899	0.143	-0.373	-1.6902	0.9996	670	
4	9	1	7.546	7.638	7.629	-0.404	-0.092	-0.4055	0.9997	671	
4	9	0	12.790	12.824	-12.830	-0.129	-0.034	-0.1594	0.9989	672	
4	10	0	25.341	24.420	24.214	3.535	0.921	5.0364	0.9959	673	
4	10	1	27.945	27.422	27.376	2.425	0.523	2.8636	0.9956	674	
4	10	2	30.892	32.009	31.869	3.751	-1.117	-6.1406	0.9950	675	
4	10	3	19.974	19.934	-19.821	-2.280	0.041	0.2125	0.9982	676	
4	10	4	22.191	22.744	22.514	3.406	-0.553	-2.7964	0.9977	677	
4	10	5	25.379	25.986	25.921	2.347	-0.606	-2.9949	0.9968	678	
4	10	6	26.125	26.798	26.620	3.477	-0.673	-3.1222	0.9964	679	
4	10	7	12.010	12.035	-11.878	-1.964	-0.025	-0.0989	0.9992	680	
4	11	7	13.978	14.615	-14.605	-0.734	-0.636	-2.5857	0.9989	681	
4	11	6	1.470 *	1.392	1.389	-0.085	0.079	0.0714	1.0000	682	* **
4	11	5	15.653	16.451	16.439	0.855	-0.798	-3.6092	0.9987	683	
4	11	4	5.332	5.320	5.318	0.171	0.012	0.0365	0.9999	684	
4	11	3	19.956	20.710	-20.713	-0.846	-0.754	-3.8356	0.9980	685	
4	11	2	5.257	4.733	4.732	-0.074	0.525	1.7271	0.9999	686	
4	11	1	21.496	21.676	21.688	0.889	-0.179	-0.9343	0.9972	687	

CYCLE THREE.

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
4	11	0	6.947	8.089	8.089	0.189	-1.143	-4.0785	0.9995	690	
4	12	0	30.949	30.466	30.435	2.865	0.483	2.4411	0.9932	691	
4	12	1	25.886	24.721	-24.669	-2.204	1.165	5.8928	0.9963	692	
4	12	2	43.946	44.011	44.029	4.255	-0.064	-0.3308	0.9899	693	
4	12	3	25.920	25.254	25.194	2.236	0.666	3.3122	0.9969	694	
4	12	4	24.507	25.152	25.040	2.742	-0.646	-3.1100	0.9970	695	
4	12	5	19.035	18.929	-18.842	-1.982	0.106	0.4792	0.9983	696	
4	12	6	30.829	31.661	31.504	3.896	-0.832	-3.7977	0.9948	697	
4	13	4	3.990	1.741	1.741	0.002	2.249	5.4791	1.0000	699	
4	13	3	1.391 *	0.546	-0.306	0.453	0.844	0.8081	1.0000	700	* **
4	13	2	7.931	7.683	-7.685	0.010	0.247	0.9195	0.9997	701	
4	13	1	3.175	2.788	-2.750	-0.456	0.387	0.8112	1.0000	702	
4	13	0	5.013	1.460	1.460	-0.007	3.553	10.0858	1.0000	703	
4	14	0	36.591	36.762	36.654	4.646	-0.170	-0.8086	0.9900	704	
4	14	1	11.001	11.064	10.905	1.896	-0.062	-0.2482	0.9992	705	
4	14	2	12.998	12.955	12.802	2.029	0.042	0.1762	0.9990	706	
4	14	3	14.450	14.694	-14.592	-1.807	-0.245	-1.0692	0.9988	707	
4	14	4	32.388	33.489	33.291	4.460	-1.102	-5.0667	0.9941	708	
4	15	3	6.949	7.661	7.661	-0.126	-0.713	-2.2554	0.9957	709	
4	15	2	6.311	6.677	-6.660	-0.489	-0.366	-1.0831	0.9997	710	
4	15	1	4.250	4.511	-4.508	0.180	-0.261	-0.6229	0.9999	711	
4	15	0	3.085	3.124	3.081	0.518	-0.039	-0.0664	0.9999	712	
4	16	0	4.730	5.382	5.172	1.490	-0.652	-1.5150	0.9998	713	
4	16	1	12.093	12.445	-12.382	-1.311	-0.352	-1.3768	0.9989	714	
5	14	3	3.400	3.739	-3.716	-0.413	-0.338	-0.6344	0.9999	715	
5	14	2	5.642	5.550	5.504	0.714	0.093	0.2626	0.9998	716	
5	14	1	5.616	5.259	5.239	0.462	0.357	1.0197	0.9998	717	
5	14	0	17.238	16.360	-16.360	-0.736	0.877	3.7497	0.9981	718	
5	13	0	6.824	6.725	6.583	1.380	0.099	0.3111	0.9997	719	
5	13	1	3.384	2.958	2.857	0.768	0.426	0.8952	0.9999	720	
5	13	2	33.066	33.678	33.395	5.123	-0.611	-2.8316	0.9937	721	
5	13	3	1.439 *	0.894	0.606	-0.658	0.545	0.5044	1.0000	722	* **
5	13	4	6.786	7.422	7.300	1.344	-0.636	-2.0064	0.9997	723	
5	12	5	6.328	6.858	-6.892	-0.296	-0.570	-1.7151	0.9998	724	
5	12	4	1.480 *	1.436	1.338	0.521	0.044	0.0397	1.0000	725	* **
5	12	3	1.406 *	0.445	0.305	0.325	0.960	0.9103	1.0000	726	* **
5	12	2	3.410	2.202	2.152	-0.467	1.208	2.7591	1.0000	727	
5	12	1	4.038	4.939	-4.929	-0.326	-0.901	-1.9806	0.9999	728	
5	12	0	1.452 *	1.700	1.609	0.548	-0.248	-0.2273	1.0000	729	* **
5	11	0	63.479	62.411	63.012	5.911	1.068	5.3454	0.9725	730	
5	11	1	4.760	3.676	-3.662	-0.316	1.084	3.2232	0.9999	731	
5	11	2	8.628	8.135	-8.073	1.013	0.493	1.9241	0.9997	732	
5	11	3	1.407 *	1.001	-0.940	0.343	0.407	0.3852	1.0000	733	* **
5	11	4	54.901	55.874	55.999	5.670	-0.973	-4.7349	0.9854	734	
5	11	5	6.875	6.200	-6.196	-0.257	0.675	2.2615	0.9998	735	
5	10	6	6.366	6.558	6.529	0.618	-0.192	-0.5800	0.9998	736	
5	10	5	3.470	1.774	1.771	-0.096	1.696	2.9863	1.0000	739	
5	10	4	3.138	1.941	-1.853	-0.576	1.197	2.4400	1.0000	740	
5	10	3	5.042	5.414	5.410	0.210	-0.372	-1.1329	0.9999	741	
5	10	2	10.122	10.702	10.683	0.693	-0.581	-2.4917	0.9995	742	
5	10	1	2.518	2.151	-2.146	-0.157	0.366	0.6436	1.0000	743	
5	10	0	1.585 *	0.723	-0.411	-0.595	0.862	0.7251	1.0000	744	* **
5	9	0	29.158	28.606	28.642	1.540	0.552	2.8965	0.9947	745	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
5	9	1	7.992	7.127	7.125	-0.206	0.865	3.5377	0.9997	746	
5	9	2	48.470	49.197	49.142	5.719	-0.727	-3.9033	0.9889	747	
5	9	3	7.299	4.793	-4.786	0.264	2.505	9.7842	0.9999	748	
5	9	4	22.615	23.228	23.209	1.478	-0.613	-2.9545	0.9976	749	
5	9	5	7.231	6.983	6.983	-0.132	0.247	0.8446	0.9998	750	
5	9	6	34.548	35.627	35.355	5.234	-1.079	-4.9994	0.9937	751	
5	8	7	1.489 *	1.315	-1.307	-0.145	0.173	0.1550	1.0000	752	* **
5	8	6	12.632	13.110	-13.090	-0.816	-0.477	-1.9800	0.9992	753	
5	8	5	6.595	6.478	6.472	0.287	0.117	0.3936	0.9998	754	
5	8	4	8.485	8.842	8.802	0.856	-0.357	-1.3946	0.9996	755	
5	8	3	1.401 *	3.161	-3.155	-0.206	-1.761	-1.6733	1.0000	756	* **
5	8	2	21.931	22.042	-22.048	-0.915	-0.111	-0.5918	0.9978	757	
5	8	1	6.529	5.853	5.848	0.260	0.675	2.6116	0.9998	758	
5	7	0	50.404	49.434	49.500	5.691	0.970	5.5492	0.9843	760	
5	7	1	23.715	22.608	22.602	1.289	1.107	6.2041	0.9973	761	
5	7	2	11.947	11.829	11.709	1.708	0.118	0.5770	0.9994	762	
5	7	3	15.844	15.725	-15.688	-1.190	0.119	0.6016	0.9989	763	
5	7	4	42.056	43.702	43.546	5.465	-1.646	-8.6631	0.9916	764	
5	7	5	21.219	21.303	21.287	1.268	-0.084	-0.4005	0.9979	765	
5	7	6	11.509	11.261	11.149	1.610	0.248	1.0026	0.9994	766	
5	7	7	8.540	8.425	-8.366	-1.011	0.115	0.4036	0.9996	767	
5	6	8	1.474 *	0.524	-0.327	-0.410	0.949	0.8586	1.0000	768	* **
5	6	7	7.977	7.037	-7.034	0.237	0.940	3.2715	0.9998	769	
5	6	6	2.579	1.160	1.057	0.477	1.419	2.3573	1.0000	770	
5	6	5	2.894	2.732	-2.723	-0.221	0.162	0.3244	1.0000	771	
5	6	4	1.329 *	0.690	0.507	-0.468	0.639	0.6403	1.0000	772	* **
5	6	3	7.991	7.684	-7.681	0.247	0.306	1.2816	0.9997	773	
5	6	2	2.433	1.799	1.721	0.525	0.634	1.3263	1.0000	774	
5	6	1	2.768	2.358	2.344	-0.248	0.411	0.9733	1.0000	775	
5	6	0	1.231 *	1.028	0.904	-0.489	0.203	0.2200	1.0000	776	* **
5	5	0	3.752	1.962	0.479	1.903	1.790	2.9139	1.0000	777	
5	5	1	31.447	31.186	-31.214	-1.790	0.261	1.5596	0.9949	778	
5	5	2	68.582	69.088	69.602	5.661	-0.505	-3.0123	0.9788	779	
5	5	3	22.482	22.690	22.648	1.750	-0.208	-1.1367	0.9977	780	
5	5	4	4.419	2.505	1.699	1.841	1.914	5.8335	1.0000	781	
5	5	5	27.524	28.185	-28.188	-1.667	-0.661	-3.1890	0.9963	784	
5	5	6	50.478	51.964	52.035	5.215	-1.486	-7.1948	0.9874	785	
5	5	7	13.429	13.439	13.353	1.576	-0.011	-0.0439	0.9991	786	
5	5	8	3.037	4.285	3.948	1.665	-1.248	-1.9166	0.9999	787	
5	4	8	1.585 *	2.983	2.970	0.275	-1.399	-1.1755	0.9999	788	* **
5	4	7	3.131	3.627	-3.580	-0.583	-0.496	-0.9073	0.9999	789	
5	4	6	1.422 *	0.637	-0.579	-0.265	0.785	0.7354	1.0000	790	* **
5	4	5	13.263	13.817	13.801	0.779	-0.553	-2.4983	0.9991	791	
5	4	4	8.047	7.735	7.728	0.342	0.312	1.3225	0.9997	792	
5	4	3	8.847	9.019	-8.993	-0.702	-0.172	-0.8029	0.9996	793	
5	4	2	4.011	3.877	3.868	-0.272	0.134	0.4273	0.9999	794	
5	4	1	14.840	14.499	14.486	0.777	0.341	1.9774	0.9989	795	
5	4	0	11.609	11.556	11.555	0.369	0.053	0.2936	0.9991	796	
5	3	0	61.636	60.749	61.280	4.974	0.887	5.6107	0.9763	797	
5	3	1	5.511	5.965	5.646	1.928	-0.454	-1.9055	0.9998	798	
5	3	2	41.730	42.903	42.985	2.875	-1.173	-7.1196	0.9918	799	
5	3	3	4.226	4.623	-4.232	-1.862	-0.397	-1.1960	0.9999	800	
5	3	4	46.404	47.929	47.953	4.758	-1.525	-8.1673	0.9893	801	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
5	3	5	4.916	5.006	4.663	1.822	-0.091	-0.2618	0.9999	802	
5	3	6	26.628	27.543	27.468	2.637	-0.916	-4.2551	0.9963	803	
5	3	7	1.543 *	2.985	-2.494	-1.641	-1.442	-1.2440	1.0000	804	* **
5	3	8	28.447	28.615	28.383	4.173	-0.168	-0.7145	0.9950	805	
5	2	8	4.790	3.827	-3.812	-0.346	0.963	2.2533	0.9999	806	
5	2	7	13.123	12.923	12.904	0.801	0.200	0.7884	0.9990	807	
5	2	6	3.746	3.097	3.075	0.368	0.649	1.4134	0.9999	808	
5	2	5	8.480	8.703	-8.676	-0.709	-0.223	-0.8441	0.9996	809	
5	2	4	12.390	12.682	-12.679	-0.423	-0.292	-1.3384	0.9992	810	
5	2	3	16.745	17.189	17.180	0.849	-0.444	-2.3109	0.9986	811	
5	2	2	1.184 *	0.702	0.591	0.379	0.482	0.5417	1.0000	812	* **
5	2	1	14.673	15.167	-15.153	-0.812	-0.494	-2.8898	0.9990	813	
5	1	0	45.179	43.554	43.669	3.686	1.625	10.4500	0.9877	815	
5	1	1	41.432	42.321	-42.423	-2.549	-0.889	-5.3948	0.9916	816	
5	1	2	32.020	33.527	33.376	4.068	-1.507	-8.6038	0.9943	817	
5	1	3	42.853	44.075	44.220	2.529	-1.222	-6.6619	0.9902	818	
5	1	4	36.262	37.306	37.270	3.549	-1.044	-5.3980	0.9929	819	
5	1	5	26.843	27.223	-27.176	-2.351	-0.380	-1.8435	0.9960	820	
5	1	6	25.657	26.289	26.071	3.761	-0.632	-2.9176	0.9961	821	
5	1	7	32.532	31.945	31.964	2.280	0.587	2.5683	0.9938	822	
5	1	8	27.410	26.711	26.579	3.165	0.699	2.9575	0.9958	823	
5	0	7	4.347	4.455	-4.432	-0.452	-0.108	-0.2413	0.9999	824	
5	0	5	9.322	8.427	-8.413	0.518	0.895	2.4357	0.9996	825	
5	0	3	2.769	1.869	-1.792	-0.529	0.900	1.7947	1.0000	826	
5	0	1	6.475	5.197	-5.169	0.545	1.278	4.8321	0.9998	827	
6	0	0	32.964	31.425	31.027	5.631	1.539	7.8991	0.9931	828	
6	0	2	26.237	26.986	26.979	1.753	-0.749	-3.5621	0.9963	829	
6	0	4	28.672	28.657	28.206	5.408	0.015	0.0658	0.9957	830	
6	0	6	23.976	23.016	22.990	1.655	0.960	3.9284	0.9971	833	
6	1	7	3.912	4.064	-4.063	0.089	-0.152	-0.2818	0.9999	834	
6	1	6	7.949	6.962	-6.915	-0.812	0.987	3.1245	0.9997	835	
6	1	5	13.124	13.480	13.486	0.078	-0.356	-1.3896	0.9991	836	
6	1	4	15.586	16.364	16.349	0.911	-0.779	-3.2646	0.9987	837	
6	1	3	8.298	8.185	-8.186	0.044	0.113	0.4175	0.9997	838	
6	1	2	4.886	5.300	-5.230	-0.864	-0.415	-1.1572	0.9999	839	
6	1	1	13.014	13.110	13.115	0.020	-0.097	-0.4728	0.9993	840	
6	1	0	22.208	21.685	21.692	0.967	0.523	2.7665	0.9974	841	
6	2	0	5.266	5.372	5.169	1.463	-0.106	-0.3524	0.9998	842	
6	2	1	26.495	26.301	26.320	0.974	0.194	1.0657	0.9972	843	
6	2	2	67.878	68.821	69.252	5.947	-0.943	-5.0030	0.9803	844	
6	2	3	19.712	19.912	-19.908	-0.917	-0.199	-0.9436	0.9982	845	
6	2	4	4.393	4.272	4.032	1.410	0.121	0.3009	0.9999	846	
6	2	5	23.946	23.744	23.757	0.943	0.202	0.9058	0.9973	847	
6	2	6	50.979	51.097	51.155	5.457	-0.118	-0.5279	0.9865	848	
6	2	7	12.365	11.769	-11.746	-0.798	0.596	2.1840	0.9992	849	
6	3	7	9.714	9.584	-9.582	-0.303	0.130	0.4519	0.9995	850	
6	3	6	3.139	3.129	3.069	0.609	0.010	0.0166	1.0000	851	
6	3	5	1.464 *	1.806	-1.769	0.366	-0.342	-0.3115	1.0000	852	* **
6	3	4	1.482 *	2.477	-2.398	-0.623	-0.995	-0.8949	1.0000	853	* **
6	3	3	9.333	9.359	-9.354	-0.364	-0.026	-0.1027	0.9996	854	
6	3	2	4.099	4.165	4.111	0.670	-0.067	-0.1870	0.9999	855	
6	3	1	3.682	3.487	3.466	0.379	0.195	0.5226	0.9999	856	
6	3	0	3.174	2.619	-2.537	-0.652	0.555	1.2419	1.0000	857	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
6	4	0	72.660		70.222	71.001	5.728	2.438	13.4736	0.9718	858	
6	4	1	5.015		3.047	-2.847	-1.085	1.968	6.1685	1.0000	859	
6	4	2	5.147		4.755	4.461	1.647	0.392	1.3392	0.9999	860	
6	4	3	1.427	*	1.318	-0.779	1.064	0.109	0.1017	1.0000	861	* **
6	4	4	58.730		59.809	60.039	5.487	-1.079	-5.3826	0.9841	862	
6	4	5	4.659		5.234	-5.137	-1.006	-0.575	-1.3856	0.9999	863	
6	4	6	1.555	*	3.325	2.954	1.527	-1.770	-1.5161	0.9999	864	* **
6	4	7	3.657		1.886	-1.624	0.960	1.770	3.6090	1.0000	865	
6	5	7	13.682		13.496	13.483	0.720	0.186	0.7386	0.9991	866	
6	5	6	3.839		4.570	-4.538	-0.546	-0.731	-1.4889	0.9999	867	
6	5	5	9.896		9.953	-9.936	-0.612	-0.057	-0.2243	0.9995	868	
6	5	4	2.870		2.642	-2.583	0.556	0.227	0.4253	1.0000	869	
6	5	3	16.765		16.688	16.681	0.754	0.076	0.3809	0.9988	870	
6	5	2	9.762		10.408	-10.391	-0.624	-0.646	-2.8105	0.9995	871	
6	5	1	15.332		15.052	-15.043	-0.712	0.280	1.3995	0.9989	872	
6	5	0	5.756		5.196	-5.165	0.568	0.560	1.8653	0.9998	873	
6	6	0	31.095		30.698	30.680	2.540	0.397	2.0409	0.9943	874	
6	6	2	20.304		21.077	20.601	4.547	-0.772	-3.8524	0.9981	876	
6	6	3	8.746		8.639	-8.497	-1.566	0.108	0.4376	0.9997	877	
6	6	4	27.331		28.178	28.120	2.456	-0.847	-4.1380	0.9965	878	
6	6	5	6.881		7.412	7.247	1.562	-0.532	-1.7709	0.9997	879	
6	6	6	19.671		19.633	19.197	4.201	0.038	0.1601	0.9981	882	
6	7	6	12.663		12.569	12.565	0.491	0.094	0.3731	0.9992	883	
6	7	5	3.285		3.316	3.246	0.679	-0.032	-0.0595	0.9999	884	
6	7	4	7.671		8.136	-8.125	-0.442	-0.465	-1.6669	0.9997	885	
6	7	3	3.647		4.200	4.159	-0.582	-0.553	-1.2362	0.9999	886	
6	7	2	19.297		19.386	19.394	0.557	-0.089	-0.4392	0.9983	887	
6	7	1	1.379	*	0.664	0.044	0.663	0.715	0.6904	1.0000	888	* **
6	7	0	7.785		7.518	-7.505	-0.451	0.268	0.9916	0.9997	889	
6	8	0	40.705		39.993	39.971	4.224	0.712	3.5604	0.9900	890	
6	8	1	35.918		35.489	-35.530	-2.309	0.429	2.1543	0.9935	891	
6	8	2	20.754		21.749	21.595	2.774	-0.995	-4.7886	0.9979	892	
6	8	3	36.920		37.097	37.136	2.329	-0.176	-0.8758	0.9940	893	
6	8	4	34.037		34.999	34.861	4.050	-0.962	-4.6291	0.9945	894	
6	8	5	25.141		25.881	-25.838	-2.094	-0.740	-3.3582	0.9968	895	
6	8	6	15.703		16.801	16.617	2.559	-1.098	-4.5421	0.9986	896	
6	9	5	11.470		11.708	-11.691	-0.696	-0.237	-0.9309	0.9993	897	
6	9	4	3.159		3.305	-3.305	0.060	-0.146	-0.2787	0.9999	898	
6	9	3	3.248		3.743	3.667	0.749	-0.494	-0.9360	0.9999	899	
6	9	2	7.243		7.322	7.322	0.006	-0.079	-0.2842	0.9998	900	
6	9	1	8.531		9.205	-9.176	-0.759	-0.674	-2.5651	0.9995	901	
6	9	0	4.491		3.357	-3.357	0.065	1.133	2.9752	0.9999	902	
6	10	0	17.995		17.812	17.560	3.097	0.184	0.8139	0.9979	903	
6	10	1	13.879		12.671	12.520	1.985	1.208	5.2837	0.9991	904	
6	10	2	40.486		40.883	40.887	3.661	-0.397	-1.9129	0.9919	905	
6	10	3	13.831		14.301	-14.181	-1.901	-0.470	-2.0425	0.9990	906	
6	10	4	14.835		15.645	15.370	2.969	-0.811	-3.4682	0.9989	907	
6	10	5	9.064		9.170	8.974	1.894	-0.106	-0.3913	0.9996	908	
6	11	4	1.414	*	0.340	-0.309	0.142	1.074	1.0122	1.0000	909	* **
6	11	3	8.114		8.271	-8.232	-0.818	-0.157	-0.5658	0.9997	910	
6	11	2	10.031		10.452	-10.454	-0.163	-0.421	-1.5852	0.9994	911	
6	11	1	10.677		10.385	10.350	0.885	0.292	1.1671	0.9994	912	
6	11	0	1.578	*	2.308	-2.304	0.134	-0.730	-0.6159	1.0000	913	* **

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
6	12	0	6.401	6.251	5.760	2.432	0.149	0.4678	0.9997	914	
6	12	1	5.913	5.868	-5.615	-1.707	0.045	0.1311	0.9998	915	
6	12	2	31.386	32.164	32.016	3.926	-0.778	-3.5387	0.9943	916	
6	12	3	4.921	5.421	5.139	1.730	-0.501	-1.3073	0.9998	917	
6	13	1	4.486	4.101	-4.051	-0.646	0.384	0.8986	0.9999	918	
6	13	0	11.469	11.050	11.053	-0.139	0.419	1.3278	0.9991	919	
7	10	2	3.733	3.391	3.280	0.861	0.342	0.7231	0.9999	920	
7	10	1	3.389	3.026	-3.026	-0.001	0.363	0.6596	0.9999	921	
7	10	0	8.943	8.124	-8.082	-0.847	0.819	2.7520	0.9995	922	
7	9	0	1.532 *	1.853	1.189	1.422	-0.322	-0.2798	1.0000	923	* **
7	9	1	4.206	3.307	3.305	-0.116	0.899	2.0134	0.9999	924	
7	9	2	32.233	32.405	32.112	4.921	-0.172	-0.7891	0.9950	925	
7	9	3	4.487	3.788	-3.785	0.155	0.699	1.8291	0.9999	926	
7	8	4	10.412	10.815	10.785	0.837	-0.403	-1.4992	0.9994	927	
7	8	3	1.469 *	2.189	-2.176	-0.241	-0.720	-0.6530	1.0000	928	* **
7	8	2	5.650	5.681	-5.627	-0.781	-0.031	-0.0936	0.9999	931	
7	8	1	1.480 *	1.613	1.587	0.287	-0.132	-0.1191	1.0000	932	* **
7	7	0	39.833	38.790	38.649	4.960	1.043	4.8543	0.9910	934	
7	7	1	17.574	17.008	16.981	1.155	0.566	2.5419	0.9986	935	
7	7	2	22.231	22.648	22.603	1.790	-0.417	-1.9471	0.9977	936	
7	7	3	19.841	19.833	-19.819	-1.118	0.008	0.0375	0.9982	937	
7	7	4	33.176	33.936	33.695	4.746	-0.760	-3.4464	0.9946	938	
7	6	5	1.508 *	0.914	0.806	-0.429	0.595	0.5256	1.0000	939	* **
7	6	4	6.194	6.076	-6.037	-0.688	0.119	0.3592	0.9998	940	
7	6	3	5.177	5.108	5.076	0.577	0.069	0.1743	0.9999	941	
7	6	2	5.759	6.221	6.177	0.745	-0.462	-1.3285	0.9998	942	
7	6	1	3.781	2.220	-2.157	-0.524	1.561	3.5803	1.0000	943	
7	6	0	7.205	6.957	-6.920	-0.721	0.248	0.8510	0.9997	944	
7	5	0	8.624	8.352	8.160	1.788	0.272	1.0363	0.9996	945	
7	5	1	9.368	8.641	-8.523	-1.434	0.727	2.9051	0.9997	946	
7	5	2	50.577	51.274	51.312	5.062	-0.696	-3.4121	0.9889	947	
7	5	3	13.576	13.634	13.560	1.466	-0.058	-0.2517	0.9992	948	
7	5	4	7.244	7.354	7.152	1.718	-0.110	-0.3521	0.9998	949	
7	5	5	3.594	2.764	-2.448	-1.283	0.830	1.6693	1.0000	950	
7	4	5	6.062	6.264	6.220	0.740	-0.202	-0.5381	0.9998	951	
7	4	4	1.479 *	0.612	-0.343	0.507	0.866	0.7801	1.0000	952	* **
7	4	3	9.385	9.147	-9.122	-0.697	0.239	0.9184	0.9996	953	
7	4	2	5.155	5.072	-5.044	-0.533	0.083	0.2384	0.9999	954	
7	4	1	8.372	8.415	8.383	0.752	-0.042	-0.1702	0.9997	955	
7	4	0	1.427 *	1.306	-1.196	0.524	0.122	0.1136	1.0000	956	* **
7	3	0	30.703	29.460	29.214	4.307	1.243	6.0844	0.9953	957	
7	3	1	12.076	11.654	11.550	1.578	0.421	1.9129	0.9994	958	
7	3	2	11.226	11.575	11.295	2.543	-0.349	-1.4497	0.9995	959	
7	3	3	11.118	11.528	-11.430	-1.527	-0.410	-1.5555	0.9994	960	
7	3	4	27.635	28.467	28.216	4.148	-0.832	-3.6647	0.9963	961	
7	3	5	10.584	10.264	10.158	1.488	0.320	1.1424	0.9995	962	
7	2	6	5.650	5.918	5.912	0.273	-0.268	-0.6646	0.9998	963	
7	2	5	7.769	8.209	-8.174	-0.769	-0.440	-1.2974	0.9997	964	
7	2	4	1.599 *	2.712	-2.700	-0.252	-1.113	-0.9265	1.0000	965	* **
7	2	3	7.461	7.393	7.341	0.886	0.068	0.2256	0.9998	966	
7	2	2	8.807	9.051	9.047	0.310	-0.244	-0.9213	0.9997	967	
7	2	1	8.672	8.957	-8.917	-0.866	-0.285	-1.1221	0.9997	968	
7	2	0	2.575	1.921	-1.904	-0.257	0.654	1.1400	1.0000	969	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR		
7	1	0	45.309	44.069	44.158	3.480	1.240	6.2062	0.9898	970	
7	1	1	24.224	24.674	-24.609	-2.159	-0.450	-2.0956	0.9976	971	
7	1	2	23.272	23.487	23.242	3.571	-0.215	-0.9504	0.9976	972	
7	1	3	17.936	17.670	17.560	2.083	0.265	1.1124	0.9986	973	
7	1	4	36.732	37.550	37.528	3.336	-0.818	-3.5269	0.9933	974	
7	1	5	24.052	23.997	-23.945	-2.038	0.055	0.2234	0.9971	975	
7	1	6	18.627	17.864	17.577	3.279	0.763	2.9680	0.9983	976	
7	0	5	9.355	9.360	9.314	0.954	-0.005	-0.0155	0.9995	977	
7	0	3	4.654	4.356	-4.269	-0.866	0.299	0.6234	0.9999	980	
7	0	1	8.538	8.314	8.261	0.955	0.224	0.7484	0.9997	981	
8	0	0	39.355	36.565	36.392	4.912	2.790	11.8617	0.9915	982	
8	0	2	16.599	17.147	17.076	1.679	-0.547	-1.9472	0.9986	983	
8	1	3	10.412	10.092	10.089	0.330	0.320	0.9943	0.9995	984	
8	1	2	10.428	10.615	-10.580	-0.901	-0.187	-0.6142	0.9995	985	
8	1	1	13.915	13.385	-13.386	-0.305	0.530	2.1090	0.9993	986	
8	1	0	1.900 *	2.387	-2.237	0.832	-0.486	-0.3407	1.0000	987	* **
8	2	0	6.700	6.559	6.396	1.457	0.141	0.4077	0.9998	988	
8	2	1	9.643	10.003	9.977	0.748	-0.360	-1.2949	0.9996	989	
8	2	2	39.691	39.396	39.210	5.025	0.295	1.2879	0.9932	990	
8	2	3	10.987	10.644	-10.622	-0.730	0.343	1.1798	0.9995	991	
8	3	3	1.550 *	1.511	1.465	-0.373	0.038	0.0331	1.0000	992	* **
8	3	2	11.836	11.423	11.383	0.990	0.413	1.5716	0.9994	993	
8	3	0	14.084	12.879	-12.847	-0.989	1.205	4.8154	0.9991	995	
8	4	0	40.994	39.072	38.940	4.841	1.923	8.7005	0.9915	996	
8	4	1	5.235	4.176	-4.082	-0.884	1.059	2.6479	0.9999	997	
8	4	2	5.837	6.382	6.179	1.599	-0.545	-1.5100	0.9998	998	
8	4	3	6.214	5.608	5.536	0.896	0.606	1.6769	0.9999	999	
8	5	2	1.500 *	1.285	-1.135	-0.603	0.215	0.1909	1.0000	1000	* **
8	5	1	4.673	2.875	2.832	-0.495	1.798	4.5549	1.0000	1001	
8	5	0	15.162	15.012	15.004	0.734	0.150	0.6085	0.9987	1002	
8	6	0	22.507	21.477	21.381	2.317	1.031	4.4234	0.9973	1003	
8	6	1	10.306	9.384	9.290	1.342	0.922	3.4227	0.9996	1004	

All reflections: $R = 3.2$

$R_{wtd.} = 2.6$

Unrejected Reflections: $R = 2.9$

$R_{wtd.} = 2.6$