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 'Al'  'Al'   0.0645   0.0514
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 'Si'  'Si'   0.0817   0.0704
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 'Ca'  'Ca'   0.2262   0.3064
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 'Fe'  'Fe'   0.3463   0.8444
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 'Mn'  'Mn'   0.3368   0.7283
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 'Bi'  'Bi'  -4.1077  10.2566
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary   difmap
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_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.00002(10)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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_refine_ls_wR_factor_ref         0.1113
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X1MN Mn 0.7500 0.2500 0.2500 0.0127(6) Uani 0.10(2) 4 d SP . .
X2CA Ca 0.81066(7) 0.04548(7) 0.37882(9) 0.0123(3) Uani 1.000(5) 1 d . . .
X3 Ca 0.9023(4) 0.8205(6) 0.8935(10) 0.0189(9) Uani 0.88(5) 1 d P . .
Bi3 Bi 0.9107(10) 0.8365(14) 0.8684(18) 0.012(3) Uani 0.069(11) 1 d P . .
X4 Ca 0.7500 0.7500 0.1369(6) 0.0142(17) Uani 0.515(12) 4 d SP . .
Y1MN Mn 0.7500 0.7500 0.0567(5) 0.0155(15) Uani 0.479(9) 4 d SP . .
Y2 Al 0.0000 0.0000 0.0000 0.0100(4) Uani 1 2 d S . .
Y3AL Al 0.88771(9) 0.12017(9) 0.12598(13) 0.0103(4) Uani 0.940(6) 1 d P . .
Y3MN Mn 0.88771(9) 0.12017(9) 0.12598(13) 0.0103(4) Uani 0.060(6) 1 d P . .
Z1 Si 0.2500 0.7500 0.0000 0.0087(6) Uani 1 4 d S . .
Z2 Si 0.82001(8) 0.04132(8) 0.87112(12) 0.0073(3) Uani 1 1 d . . .
Z3 Si 0.91633(9) 0.84938(9) 0.36405(12) 0.0115(3) Uani 1 1 d . . .
T1 As 0.0555(16) 0.0555(16) 0.2500 0.055(13) Uani 0.039(4) 2 d SP . .
O1 O2- 0.7797(2) 0.1730(2) 0.0852(3) 0.0124(8) Uani 1 1 d . . .
O2 O2- 0.8819(2) 0.1603(2) 0.2809(3) 0.0106(8) Uani 1 1 d . . .
O3 O2- 0.9541(2) 0.2234(2) 0.0756(3) 0.0114(8) Uani 1 1 d . . .
O4 O2- 0.9391(2) 0.1055(2) 0.4693(3) 0.0111(8) Uani 1 1 d . . .
O5 O2- 0.8284(2) 0.0125(2) 0.1793(3) 0.0141(8) Uani 1 1 d . . .
O6 O2- 0.8794(2) 0.7264(2) 0.0581(3) 0.0192(9) Uani 1 1 d . . .
O7A O2- 0.8230(16) 0.9435(7) 0.8220(12) 0.0113(12) Uiso 0.61(9) 1 d P . .
O7B O2- 0.841(2) 0.9493(11) 0.8123(17) 0.0113(12) Uiso 0.39(9) 1 d P . .
O8 O2- 0.9394(2) 0.9083(2) 0.0682(3) 0.0105(8) Uani 1 1 d . . .
O9 O2- 0.8541(2) 0.8541(2) 0.2500 0.0135(11) Uani 1 2 d S . .
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Cl Cl 0.7500 0.7500 0.844(2) 0.026(5) Uiso 0.40(5) 4 d SP . .
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X3 0.0185(14) 0.0129(17) 0.025(2) 0.0009(15) -0.0030(14) 0.0005(11)
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Y3MN 0.0108(8) 0.0120(8) 0.0083(8) 0.0001(6) 0.0008(6) 0.0004(5)
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O6 0.031(2) 0.014(2) 0.013(2) 0.0052(16) -0.0001(18) 0.0053(16)
O8 0.0113(18) 0.0122(18) 0.0081(19) 0.0000(15) 0.0021(14) 0.0014(15)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
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 used when they are defined by crystal symmetry. An approximate (isotropic)
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X1CA O2 2.514(3) . ?
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X1CA O2 2.514(3) 6 ?
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X2CA O8 2.333(3) 7_545 ?
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X3 O7A 2.433(13) . ?
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X3 O8 2.539(8) 1_556 ?
X3 O7B 2.55(2) 7_556 ?
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Z3 Bi3 3.521(18) 7_556 ?
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Z3 Bi3 4.28(3) 6_566 ?
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T1 O11 1.625(13) 7_545 ?
T1 O7B 1.78(5) 15_665 ?
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O3 Z2 T1 147.7(7) 11_666 9_656 ?
O4 Z2 T1 88.3(5) 15_666 9_656 ?
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O9 Z3 X2CA 71.76(8) . 7_655 ?
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X2CA Z3 X2CA 63.63(4) 4_665 7_655 ?
X3 Z3 X2CA 171.3(2) 7_556 7_655 ?
X2CA Z3 X2CA 117.30(5) 1_565 7_655 ?
Bi3 Z3 X2CA 165.5(4) 7_556 7_655 ?
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O5 Z3 X3 98.39(17) 7_655 6_566 ?
O8 Z3 X3 102.92(16) 7 6_566 ?
O9 Z3 X3 126.13(19) . 6_566 ?
X4 Z3 X3 66.81(15) 5_655 6_566 ?
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X3 Z3 X3 60.97(17) 7_556 6_566 ?
X2CA Z3 X3 122.26(10) 1_565 6_566 ?
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X2CA Z3 X3 120.41(10) 7_655 6_566 ?
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O5 Z3 Bi3 96.6(3) 7_655 6_566 ?
O8 Z3 Bi3 102.9(2) 7 6_566 ?
O9 Z3 Bi3 127.8(3) . 6_566 ?
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X2CA Z3 Bi3 56.4(2) 4_665 6_566 ?
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X2CA Z3 Bi3 123.3(2) 1_565 6_566 ?
Bi3 Z3 Bi3 61.2(4) 7_556 6_566 ?
X2CA Z3 Bi3 119.3(2) 7_655 6_566 ?
X3 Z3 Bi3 2.1(3) 6_566 6_566 ?
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O11 T1 O7B 105.7(7) 1_455 15_665 ?
O11 T1 O7B 100.2(6) 7_545 15_665 ?
O11 T1 O7B 100.2(6) 1_455 9_666 ?
O11 T1 O7B 105.7(7) 7_545 9_666 ?
O7B T1 O7B 104(2) 15_665 9_666 ?
O11 T1 O7A 107.1(6) 1_455 15_665 ?
O11 T1 O7A 100.3(6) 7_545 15_665 ?
O7B T1 O7A 2.8(7) 15_665 15_665 ?
O7B T1 O7A 101.6(18) 9_666 15_665 ?
O11 T1 O7A 100.3(6) 1_455 9_666 ?
O11 T1 O7A 107.1(6) 7_545 9_666 ?
O7B T1 O7A 101.6(18) 15_665 9_666 ?
O7B T1 O7A 2.8(7) 9_666 9_666 ?
O7A T1 O7A 98.8(16) 15_665 9_666 ?
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O11 T1 Bi3 65.4(6) 7_545 15_665 ?
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O7B T1 Bi3 65.4(11) 9_666 15_665 ?
O7A T1 Bi3 61.8(9) 15_665 15_665 ?
O7A T1 Bi3 64.4(9) 9_666 15_665 ?
O11 T1 Bi3 65.4(6) 1_455 9_666 ?
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O7B T1 Bi3 65.4(11) 15_665 9_666 ?

O7B T1 Bi3 64.1(11) 9_666 9_666 ?
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O7A T1 Bi3 61.8(9) 9_666 9_666 ?
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O11 T1 X3 65.1(6) 7_545 15_665 ?
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O7A T1 X3 66.0(8) 9_666 15_665 ?
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Bi3 T1 X3 92.2(12) 9_666 15_665 ?
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O11 T1 X3 157.6(17) 7_545 9_666 ?
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O7A T1 X3 66.0(8) 15_665 9_666 ?
O7A T1 X3 60.5(7) 9_666 9_666 ?
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O7B T1 Z2 136.0(17) 9_666 15_565 ?
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O7A T1 Z2 133.2(15) 9_666 15_565 ?
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O11 T1 Z2 94.53(19) 7_545 9_656 ?
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X3 T1 Z2 84.1(5) 9_666 9_656 ?
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X1CA O2 X3 125.39(19) . 9_766 ?
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Z2 O4 Y3MN 131.7(2) 15_665 15_666 ?
Y2 O4 Y3MN 95.52(14) 7_655 15_666 ?
Z2 O4 Y3AL 131.7(2) 15_665 15_666 ?
Y2 O4 Y3AL 95.52(14) 7_655 15_666 ?
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Y2 O4 Bi3 62.5(2) 7_655 15_765 ?
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Y3AL O4 Bi3 135.4(4) 15_666 15_765 ?
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Y3AL O4 X3 130.0(2) 15_666 15_765 ?
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Y3AL O4 Bi3 54.8(3) 15_666 7_546 ?
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X4 O6 Bi3 102.3(5) . 4_564 ?
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T1 O7A Bi3 61.4(9) 9_666 7_556 ?
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O7B O7A X3 85(4) . . ?
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O7B O7A Bi3 169(4) . 3_655 ?
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Bi3 O7A Bi3 112.9(14) . 3_655 ?
Bi3 O7A Bi3 104.3(8) 7_556 3_655 ?
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X3 O7A Bi3 8.8(4) 3_655 3_655 ?
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Bi3 O7A X3 6.2(5) 7_556 7_556 ?
X3 O7A X3 98.6(5) . 7_556 ?
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Bi3 O7B X3 103.4(12) 7_556 3_655 ?
X3 O7B X3 90.2(11) . 3_655 ?
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O7A O7B Bi3 10(4) . 3_655 ?
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T1 O7B Bi3 162.0(12) 9_666 3_655 ?
Bi3 O7B Bi3 103.9(17) . 3_655 ?
Bi3 O7B Bi3 97.7(11) 7_556 3_655 ?
X3 O7B Bi3 96.6(13) . 3_655 ?
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X3 O7B Bi3 7.9(3) 3_655 3_655 ?
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Y2 O8 X2CA 104.65(15) 1_665 7_655 ?
Z3 O8 X3 104.1(3) 7 1_554 ?
Y2 O8 X3 100.2(3) 1_665 1_554 ?
X2CA O8 X3 91.5(2) 7_655 1_554 ?
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Y2 O8 Bi3 91.5(6) 1_665 1_554 ?
X2CA O8 Bi3 94.7(3) 7_655 1_554 ?
X3 O8 Bi3 8.7(4) 1_554 1_554 ?
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Z3 O9 X4 85.68(16) 7 . ?
Z3 O9 X4 137.5(2) . . ?
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X3 O10 Bi3 125.9(11) . 8_666 ?
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Bi3 O10 Bi3 64.8(7) 4_565 8_666 ?
Bi3 O10 Bi3 109.6(10) 3_655 8_666 ?
Bi3 O10 Bi3 122.1(12) . 8_666 ?
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X3 Cl Bi3 161.4(12) . 2_665 ?
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Cl Cl Bi3 95.7(7) 5_656 . ?
Y1MN Cl Bi3 84.3(7) 1_556 . ?
X3 Cl Bi3 161.4(12) 2_665 . ?
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X3 Cl Bi3 92.1(4) 4_565 . ?
X3 Cl Bi3 7.6(3) . . ?
Bi3 Cl Bi3 168.5(14) 2_665 . ?
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Bi3 Cl Bi3 89.43(14) 4_565 . ?
O10 Cl X4 0.00(4) . 1_556 ?
Cl Cl X4 180.000(5) 5_656 1_556 ?
Y1MN Cl X4 0.000(1) 1_556 1_556 ?
X3 Cl X4 77.5(6) 2_665 1_556 ?
X3 Cl X4 77.5(6) 3_655 1_556 ?
X3 Cl X4 77.5(6) 4_565 1_556 ?
X3 Cl X4 77.5(6) . 1_556 ?
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Bi3 Cl X4 84.3(7) . 1_556 ?
T1 O11 Y2 131.9(2) 1_655 1_655 ?
T1 O11 Y3AL 124.8(2) 1_655 . ?
Y2 O11 Y3AL 102.27(16) 1_655 . ?
T1 O11 Bi3 71.4(13) 1_655 9_766 ?
Y2 O11 Bi3 109.6(5) 1_655 9_766 ?
Y3AL O11 Bi3 103.3(4) . 9_766 ?
T1 O11 X3 78.1(12) 1_655 9_766 ?
Y2 O11 X3 104.0(3) 1_655 9_766 ?
Y3AL O11 X3 101.1(2) . 9_766 ?
Bi3 O11 X3 6.9(5) 9_766 9_766 ?
T1 O11 Bi3 13.3(12) 1_655 15_765 ?
Y2 O11 Bi3 131.3(2) 1_655 15_765 ?
Y3AL O11 Bi3 126.1(2) . 15_765 ?
Bi3 O11 Bi3 58.2(6) 9_766 15_765 ?
X3 O11 Bi3 64.87(18) 9_766 15_765 ?

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_refine_diff_density_rms 0.202