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data_vii

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 'Mg'  'Mg'   0.0486   0.0363
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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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 'y, -x+1/2, z'
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_refine_special_details
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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
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.00000(4)
_refine_ls_extinction_expression
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X1MN Mn 0.7500 0.2500 0.2500 0.01045(10) Uani 0.121(7) 4 d SP . .
X2CA Ca 0.810436(14) 0.045686(14) 0.379089(18) 0.00884(6) Uani 0.961(4) 1 d P . .
X2MN Mn 0.810436(14) 0.045686(14) 0.379089(18) 0.00884(6) Uani 0.039(4) 1 d P . .
X3 Ca 0.90003(5) 0.82040(9) 0.8937(2) 0.0151(2) Uani 0.982(10) 1 d P . .
Bi3 Bi 0.9100(8) 0.8368(11) 0.8658(12) 0.010(2) Uani 0.015(2) 1 d P . .
X4 Ca 0.7500 0.7500 0.14124(8) 0.0116(3) Uani 0.505(3) 4 d SP . .
Y1A Mn 0.7500 0.7500 0.06105(16) 0.0075(2) Uiso 0.2229(10) 4 d SP . .
Y1 Fe 0.7500 0.7500 0.04018(15) 0.0075(2) Uiso 0.2229(10) 4 d SP . .
Y2 Al 0.0000 0.0000 0.0000 0.00788(9) Uani 1 2 d S . .
Y3AL Al 0.88896(2) 0.12004(2) 0.12631(3) 0.00786(10) Uani 0.909(2) 1 d P . .
Y3MN Mn 0.88896(2) 0.12004(2) 0.12631(3) 0.00786(10) Uani 0.091(2) 1 d P . .
Z1 Si 0.2500 0.7500 0.0000 0.00688(10) Uani 1 4 d S . .
Z2 Si 0.820208(19) 0.040952(19) 0.87104(2) 0.00628(6) Uani 1 1 d . . .
Z3 Si 0.91611(2) 0.84959(2) 0.36419(3) 0.00809(7) Uani 1 1 d . . .
T1 As 0.0565(2) 0.0565(2) 0.2500 0.0100(14) Uani 0.0334(10) 2 d SP . .
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O2 O2- 0.88172(5) 0.16035(5) 0.28043(7) 0.00970(14) Uani 1 1 d . . .
O3 O2- 0.95478(6) 0.22343(5) 0.07585(7) 0.01054(15) Uani 1 1 d . . .
O4 O2- 0.93917(5) 0.10559(5) 0.46983(7) 0.00873(14) Uani 1 1 d . . .
O5 O2- 0.82863(5) 0.01285(6) 0.17928(7) 0.01184(15) Uani 1 1 d . . .
O6 O2- 0.87897(7) 0.72567(6) 0.05563(8) 0.01579(17) Uani 1 1 d . . .
O7A O2- 0.8233(3) 0.94365(12) 0.8213(2) 0.0093(2) Uiso 0.564(12) 1 d P . .
O7B O2- 0.8421(3) 0.94761(16) 0.8110(3) 0.0093(2) Uiso 0.436(12) 1 d P . .
O8 O2- 0.93986(5) 0.90809(5) 0.06794(7) 0.00873(14) Uani 1 1 d . . .
O9 O2- 0.85352(5) 0.85352(5) 0.2500 0.0117(2) Uani 1 2 d S . .
O10 O2- 0.7500 0.7500 0.8669(5) 0.0183(6) Uiso 1.01(2) 4 d SP . .
Cl Cl 0.7500 0.7500 0.831(2) 0.020(5) Uiso 0.064(11) 4 d SP . .
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X2MN 0.00763(10) 0.01038(10) 0.00850(10) 0.00018(7) -0.00083(6) 0.00081(7)
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Y3MN 0.00754(15) 0.00825(15) 0.00779(16) -0.00004(10) 0.00032(10) 0.00017(10)
Z1 0.00709(15) 0.00709(15) 0.0065(2) 0.000 0.000 0.000
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O5 0.0110(4) 0.0148(4) 0.0097(3) -0.0010(3) 0.0011(3) 0.0052(3)
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O9 0.0137(3) 0.0137(3) 0.0078(5) 0.0012(3) -0.0012(3) -0.0038(4)
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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
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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X1CA O2 2.5090(8) . ?
X1CA O2 2.5090(8) 5_655 ?
X1CA O2 2.5090(8) 6 ?
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X1CA Y3AL 3.3038(4) 6 ?
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X1CA Y3AL 3.3038(4) 2_655 ?
X1CA Y3MN 3.3038(4) 2_655 ?
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X2CA Z3 3.2140(4) 3_645 ?
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Y2 Bi3 3.306(13) 9_666 ?
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O7B Bi3 O7A 84.8(6) 7_556 . ?
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O7A Bi3 Y3AL 79.8(5) 7_556 9_766 ?
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Cl Bi3 Y3AL 162.4(3) . 9_766 ?
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O7B Bi3 Y3MN 75.8(5) 7_556 9_766 ?
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O7A Bi3 Y3MN 79.8(5) 7_556 9_766 ?
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O7A Bi3 Y2 78.1(4) . 1_666 ?
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Cl Bi3 Y2 143.1(4) . 1_666 ?
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Bi3 Bi3 Y2 106.7(3) 7_556 1_666 ?
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O7B Bi3 X2CA 129.1(5) 7_556 7_656 ?
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O7A Bi3 X2CA 130.2(4) 7_556 7_656 ?
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O8 Y2 X2CA 42.12(2) 1_445 7_545 ?
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O4 Y2 X2CA 46.32(2) 7_545 7_545 ?
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X2CA Y2 O7B 77.35(4) 15_565 1_444 ?
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O11 Y2 O7B 48.28(8) 1_455 9_666 ?
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O8 Y2 O7B 105.21(7) 1_445 9_666 ?
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Bi3 Y2 O7B 36.81(18) 9_666 9_666 ?
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O8 Y2 X3 133.42(5) 9_665 1_444 ?
O8 Y2 X3 46.58(5) 1_445 1_444 ?
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O5 Y3AL O7B 107.17(7) . 15_765 ?
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O1 Z1 X1MN 52.05(3) 4_565 3 ?
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O1 Z1 X2CA 109.18(3) 9_665 14_665 ?
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X1CA Z1 X2CA 66.787(4) 9_665 14_665 ?
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X1MN Z1 X2CA 113.213(4) 3 14_665 ?

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O1 Z1 X2CA 109.18(3) 4_565 8_565 ?
O1 Z1 X2CA 133.54(3) 9_665 8_565 ?
X1MN Z1 X2CA 113.213(4) 9_665 8_565 ?
X1CA Z1 X2CA 113.213(4) 9_665 8_565 ?
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X1MN Z1 X2CA 66.787(4) 3 8_565 ?
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X1MN Z1 X2CA 66.787(4) 3 7 ?
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O2 Z2 Bi3 126.9(4) 15_666 3_645 ?
O7B Z2 Bi3 65.6(3) 1_545 3_645 ?
O4 Z2 Bi3 131.6(4) 15_666 3_645 ?
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O7B Z2 O7B 62.4(2) 1_545 5_646 ?
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O11 T1 O7B 100.48(10) 7_545 15_665 ?
O11 T1 O7B 100.48(10) 1_455 9_666 ?
O11 T1 O7B 106.24(10) 7_545 9_666 ?
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O11 T1 O7A 107.24(10) 7_545 9_666 ?
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O11 T1 Bi3 157.6(3) 7_545 9_666 ?
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O7B T1 Bi3 63.8(3) 9_666 9_666 ?
O7A T1 Bi3 64.3(2) 15_665 9_666 ?
O7A T1 Bi3 62.2(2) 9_666 9_666 ?
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Bi3 T1 X3 91.7(3) 9_666 15_665 ?
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Bi3 T1 X3 91.7(3) 15_665 9_666 ?
Bi3 T1 X3 2.31(17) 9_666 9_666 ?
X3 T1 X3 92.14(16) 15_665 9_666 ?
O11 T1 Z2 94.49(4) 1_455 15_565 ?
O11 T1 Z2 89.83(4) 7_545 15_565 ?
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O7B T1 Z2 136.1(3) 9_666 15_565 ?
O7A T1 Z2 34.40(6) 15_665 15_565 ?
O7A T1 Z2 134.1(2) 9_666 15_565 ?
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Bi3 T1 Z2 85.81(19) 9_666 15_565 ?
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X3 T1 Z2 88.12(8) 9_666 15_565 ?
O11 T1 Z2 89.83(4) 1_455 9_656 ?
O11 T1 Z2 94.49(4) 7_545 9_656 ?
O7B T1 Z2 136.1(3) 15_665 9_656 ?
O7B T1 Z2 32.37(9) 9_666 9_656 ?
O7A T1 Z2 134.1(2) 15_665 9_656 ?
O7A T1 Z2 34.40(6) 9_666 9_656 ?
Bi3 T1 Z2 85.81(19) 15_665 9_656 ?
Bi3 T1 Z2 86.14(19) 9_666 9_656 ?
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X3 T1 Z2 83.87(8) 9_666 9_656 ?
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Y3AL O1 X2CA 96.77(3) . 5_655 ?
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X2MN O3 Bi3 101.2(3) 15_665 9_766 ?
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Y2 O4 Y3MN 95.18(3) 7_655 15_666 ?
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Y2 O4 O7B 93.67(9) 7_655 15_765 ?
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X3 O6 X2CA 79.51(3) 1_554 7_655 ?
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T1 O7A Bi3 61.3(5) 9_666 7_556 ?
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Bi3 O7A X3 110.6(5) 7_556 3_655 ?
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O7B O7A O7B 107.48(17) 7_556 5_656 ?
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Bi3 O7A O11 95.14(17) 3_655 . ?
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Bi3 O7B O2 98.0(3) 7_556 15_676 ?
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Z2 O7B O11 99.23(18) 1_565 15_676 ?

T1 O7B O11 35.39(10) 9_666 15_676 ?
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Bi3 O7B O11 51.3(5) 7_556 15_676 ?
X3 O7B O11 111.36(19) . 15_676 ?
X3 O7B O11 56.40(9) 7_556 15_676 ?
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T1 O7B O4 92.1(2) 9_666 15_676 ?
Bi3 O7B O4 99.8(2) . 15_676 ?
Bi3 O7B O4 148.8(5) 7_556 15_676 ?
X3 O7B O4 98.39(9) . 15_676 ?
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O11 O7B O4 98.56(15) 15_676 15_676 ?
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Bi3 O7B O7B 49.8(3) 7_556 7_556 ?
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O11 O7B O7B 56.90(7) 15_676 7_556 ?
O4 O7B O7B 125.18(12) 15_676 7_556 ?
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T1 O7B O3 146.7(2) 9_666 11_676 ?
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O11 O7B O3 124.93(10) 15_676 11_676 ?
O4 O7B O3 60.23(7) 15_676 11_676 ?
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T1 O7B X3 162.28(18) 9_666 3_655 ?
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O11 O7B X3 148.77(13) 15_676 3_655 ?
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Bi3 O7B Bi3 104.2(10) . 3_655 ?
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O2 O7B Bi3 102.4(4) 15_676 3_655 ?
O11 O7B Bi3 140.3(4) 15_676 3_655 ?
O4 O7B Bi3 105.44(19) 15_676 3_655 ?
O7B O7B Bi3 124.73(16) 7_556 3_655 ?
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O4 O7B O7A 129.08(18) 15_676 5_656 ?
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O11 O7B Y3AL 34.42(5) 15_676 15_676 ?
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O3 O7B Y3AL 90.71(6) 11_676 15_676 ?
X3 O7B Y3AL 125.11(12) 3_655 15_676 ?
Bi3 O7B Y3AL 117.2(4) 3_655 15_676 ?
O7A O7B Y3AL 93.51(10) 7_556 15_676 ?
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O7B O7B Y3AL 82.48(7) 5_656 15_676 ?
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Bi3 O7B Y3MN 66.1(3) 7_556 15_676 ?
X3 O7B Y3MN 144.8(2) . 15_676 ?
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O11 O7B Y3MN 34.42(5) 15_676 15_676 ?
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O3 O7B Y3MN 90.71(6) 11_676 15_676 ?
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Bi3 O7B Y3MN 117.2(4) 3_655 15_676 ?
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Y2 O8 X3 100.76(7) 1_665 1_554 ?
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X2MN O8 X3 92.17(4) 7_655 1_554 ?

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Y1 O10 X3 83.04(13) 1_556 2_665 ?
Y1A O10 X3 83.04(13) 1_556 2_665 ?
X3 O10 X3 166.1(3) . 2_665 ?
Cl O10 X3 96.96(13) . 3_655 ?
Y1 O10 X3 83.04(13) 1_556 3_655 ?
Y1A O10 X3 83.04(13) 1_556 3_655 ?
X3 O10 X3 89.16(3) . 3_655 ?
X3 O10 X3 89.16(3) 2_665 3_655 ?
Cl O10 X3 96.96(13) . 4_565 ?
Y1 O10 X3 83.04(13) 1_556 4_565 ?
Y1A O10 X3 83.04(13) 1_556 4_565 ?
X3 O10 X3 89.16(3) . 4_565 ?
X3 O10 X3 89.16(3) 2_665 4_565 ?
X3 O10 X3 166.1(3) 3_655 4_565 ?
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Y1 O10 Bi3 90.3(3) 1_556 . ?
Y1A O10 Bi3 90.3(3) 1_556 . ?
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