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 'Mn'  'Mn'   0.3368   0.7283
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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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P3 P 0.0352(17) 0.1305(4) 0.3659(7) 0.049(3) Uani 1 1 d . . .
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Mg Mg 0.293(3) 0.0428(8) 0.5181(12) 0.041(10) Uani 0.464(19) 1 d P . .
Zn Zn 0.293(3) 0.0428(8) 0.5181(12) 0.041(10) Uani 0.036(19) 1 d P . .
Zn1 Zn 0.2931(6) 0.18160(17) 0.5218(3) 0.0561(15) Uani 1 1 d . . .
Zn2 Zn 0.7949(6) 0.18224(15) 0.5227(2) 0.0498(14) Uani 1 1 d . . .
Fe1 Fe 0.2933(7) 0.24592(19) 0.2653(3) 0.0454(16) Uani 1 1 d . . .
Fe2 Fe 0.7899(7) 0.2456(2) 0.2650(3) 0.0473(16) Uani 1 1 d . . .
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Ca Ca 0.5369(10) 0.3734(3) 0.6401(4) 0.051(2) Uani 1 1 d . . .
O1 O 0.035(3) 0.3514(8) 0.5282(12) 0.048(6) Uani 1 1 d . . .
O2 O 0.238(3) 0.1993(8) 0.1496(12) 0.046(6) Uani 1 1 d . . .
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O5 O 0.555(3) 0.3510(10) 0.4912(13) 0.049(6) Uani 1 1 d . . .
O6 O 0.742(3) 0.2857(8) 0.3839(11) 0.039(6) Uani 1 1 d . . .
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O13 O 0.373(3) 0.1265(9) 0.6114(15) 0.073(8) Uani 1 1 d . . .
O14 O 0.544(3) 0.0826(9) 0.7455(13) 0.052(6) Uani 1 1 d . . .
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OH18 O 0.038(3) 0.3076(8) 0.2585(11) 0.050(6) Uani 1 1 d . . .
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Mg 0.023(14) 0.054(15) 0.047(16) 0.014(10) 0.018(9) 0.010(9)
Zn 0.023(14) 0.054(15) 0.047(16) 0.014(10) 0.018(9) 0.010(9)
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Zn2 0.048(3) 0.053(3) 0.048(3) -0.003(2) 0.001(2) 0.003(2)
Fe1 0.043(3) 0.051(3) 0.042(4) -0.004(2) 0.004(3) 0.004(2)
Fe2 0.047(4) 0.050(3) 0.045(4) 0.001(2) 0.002(3) 0.000(2)
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Ca 0.051(5) 0.056(5) 0.045(5) -0.001(4) 0.002(4) -0.004(4)
O1 0.055(16) 0.029(13) 0.058(16) 0.030(12) 0.011(12) 0.012(11)
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O3 0.033(15) 0.053(14) 0.048(15) 0.002(11) 0.005(13) -0.017(11)
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O14 0.043(15) 0.054(15) 0.060(16) -0.013(14) 0.013(12) 0.018(11)
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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)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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P3 O9 1.53(2) 1_455 ?
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P4 O15 1.56(2) . ?
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Mg OW24 1.99(3) 1_545 ?
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Mg OW24 2.25(3) 3_666 ?
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Mg Zn1 2.952(17) . ?
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Mg Mg 3.26(3) 3_656 ?
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Ca OW23 2.480(19) . ?
Ca O3 2.543(17) 4_566 ?
Ca Fe1 3.552(8) 4_566 ?
Ca Fe2 3.555(7) 4_566 ?
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O9 OW24 18.06(3) . ?
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O10 OW23 10.74(3) . ?
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O10 OW26 19.49(4) . ?
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O14 OW21 7.88(3) . ?
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OH17 OW21 9.20(3) . ?
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OW19 OW23 5.84(3) . ?
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OW24 Mg 1.99(3) 1_565 ?
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OW25 OW26 1.36(5) 3_566 ?
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OW26 Mg Zn 85.8(14) 1_545 3_656 ?
O12 Mg Zn 117.5(10) . 3_656 ?
OW24 Mg Zn 37.0(7) 3_666 3_656 ?
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O13 Mg Zn 111.0(11) . 3_656 ?
Zn1 Mg Zn 124.1(9) . 3_656 ?
OW25 Mg Mg 135.2(13) . 3_656 ?
OW24 Mg Mg 42.8(8) 1_545 3_656 ?
OW26 Mg Mg 85.8(14) 1_545 3_656 ?
O12 Mg Mg 117.5(10) . 3_656 ?
OW24 Mg Mg 37.0(7) 3_666 3_656 ?
O13 Mg Mg 111.0(11) . 3_656 ?
Zn1 Mg Mg 124.1(9) . 3_656 ?
Zn Mg Mg 0.0(10) 3_656 3_656 ?
O13 Zn1 O12 101.9(9) . . ?
O13 Zn1 O4 115.9(9) . . ?
O12 Zn1 O4 108.3(8) . . ?
O13 Zn1 O7 105.8(9) . . ?
O12 Zn1 O7 110.8(9) . . ?
O4 Zn1 O7 113.5(7) . . ?
O13 Zn1 Mg 52.4(8) . . ?
O12 Zn1 Mg 49.7(7) . . ?
O4 Zn1 Mg 123.6(6) . . ?
O7 Zn1 Mg 122.7(6) . . ?
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O16 Zn2 O4 107.1(9) . 1_655 ?
O9 Zn2 O4 108.4(8) . 1_655 ?
O16 Zn2 O7 112.6(9) . . ?
O9 Zn2 O7 104.6(8) . . ?
O4 Zn2 O7 114.0(7) 1_655 . ?
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O8 Fe1 O2 176.6(8) . . ?
OH17 Fe1 O2 84.3(7) . . ?
O8 Fe1 OH18 82.9(7) . . ?
OH17 Fe1 OH18 177.3(7) . . ?
O2 Fe1 OH18 97.5(7) . . ?
O8 Fe1 O11 88.6(8) . . ?
OH17 Fe1 O11 102.2(7) . . ?
O2 Fe1 O11 88.2(7) . . ?
OH18 Fe1 O11 75.9(7) . . ?
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OH17 Fe1 O15 78.5(8) . 4_565 ?
O2 Fe1 O15 93.6(7) . 4_565 ?
OH18 Fe1 O15 103.4(8) . 4_565 ?
O11 Fe1 O15 178.2(8) . 4_565 ?
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OH17 Fe1 Ca 42.0(5) . 4_565 ?
O2 Fe1 Ca 42.5(5) . 4_565 ?
OH18 Fe1 Ca 139.9(5) . 4_565 ?
O11 Fe1 Ca 100.3(6) . 4_565 ?
O15 Fe1 Ca 81.3(6) 4_565 4_565 ?
O3 Fe2 O6 179.0(8) . . ?
O3 Fe2 OH18 96.2(7) . 1_655 ?
O6 Fe2 OH18 84.2(7) . 1_655 ?
O3 Fe2 OH17 86.5(7) . . ?
O6 Fe2 OH17 93.1(7) . . ?
OH18 Fe2 OH17 177.3(7) 1_655 . ?
O3 Fe2 O15 91.7(7) . 4_565 ?

O6 Fe2 O15 89.1(7) . 4_565 ?
OH18 Fe2 O15 102.2(7) 1_655 4_565 ?
OH17 Fe2 O15 78.1(7) . 4_565 ?
O3 Fe2 O11 90.2(8) . 1_655 ?
O6 Fe2 O11 89.0(7) . 1_655 ?
OH18 Fe2 O11 76.1(7) 1_655 1_655 ?
OH17 Fe2 O11 103.5(7) . 1_655 ?
O15 Fe2 O11 177.6(8) 4_565 1_655 ?
O3 Fe2 Ca 44.5(5) . 4_565 ?
O6 Fe2 Ca 135.1(5) . 4_565 ?
OH18 Fe2 Ca 140.7(5) 1_655 4_565 ?
OH17 Fe2 Ca 42.1(5) . 4_565 ?
O15 Fe2 Ca 81.3(6) 4_565 4_565 ?
O11 Fe2 Ca 101.0(6) 1_655 4_565 ?
O1 Mn OW19 102.3(7) . . ?
O1 Mn OH18 158.2(7) . . ?
OW19 Mn OH18 96.9(7) . . ?
O1 Mn O8 96.6(7) . . ?
OW19 Mn O8 87.2(7) . . ?
OH18 Mn O8 74.0(7) . . ?
O1 Mn OW20 87.5(7) . 1_455 ?
OW19 Mn OW20 83.2(7) . 1_455 ?
OH18 Mn OW20 105.0(7) . 1_455 ?
O8 Mn OW20 170.2(7) . 1_455 ?
O1 Mn O6 91.6(7) . 1_455 ?
OW19 Mn O6 156.5(7) . 1_455 ?
OH18 Mn O6 73.9(7) . 1_455 ?
O8 Mn O6 110.1(6) . 1_455 ?
OW20 Mn O6 78.5(7) 1_455 1_455 ?
O5 Ca OW21 143.9(8) . . ?
O5 Ca OW22 71.2(7) . . ?
OW21 Ca OW22 73.0(7) . . ?
O5 Ca OH17 137.9(7) . 4_566 ?
OW21 Ca OH17 76.5(6) . 4_566 ?
OW22 Ca OH17 142.6(7) . 4_566 ?
O5 Ca O2 88.7(7) . 4_566 ?
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OW22 Ca O2 95.3(7) . 4_566 ?
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OW22 Ca Fe2 177.0(6) . 4_566 ?
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OW23 Ca Fe2 91.2(5) . 4_566 ?
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Mn O1 OW22 98.8(8) . . ?
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Fe1 O11 Fe2 98.8(8) . 1_455 ?
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Zn1 O13 Mg 88.3(10) . . ?
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OW21 O14 OW20 40.0(2) . . ?
P4 O14 OW19 14.2(7) . . ?
OW21 O14 OW19 38.7(2) . . ?
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Fe2 OH17 Ca 103.4(8) . 4_565 ?
Fe1 OH17 OW21 67.3(5) . . ?
Fe2 OH17 OW21 75.8(5) . . ?
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Fe2 OH18 Mn 102.5(8) 1_455 . ?
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Mn OW19 OW23 105.1(6) . . ?
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OW25 OW26 Zn 139(3) 3_566 1_565 ?
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Zn OW26 O16 109.9(12) 1_565 . ?
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Zn OW26 O10 130.1(12) 1_565 . ?
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_refine_diff_density_rms    0.150
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