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 'H'  'H'   0.0000   0.0000
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 'O'  'O'   0.0106   0.0060
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 'Na'  'Na'   0.0362   0.0249
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 'I'  'I'  -0.4742   1.8119
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                    6.6006(8)
_cell_length_b                    13.3561(17)
_cell_length_c                    17.888(2)
_cell_angle_alpha                 90.00
_cell_angle_beta                  93.620(7)
_cell_angle_gamma                 90.00
_cell_volume                      1573.8(3)
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_cell_measurement_reflns_used     5982
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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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_refine_ls_weighting_scheme       calc
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 'calc w=1/[\s^2^(Fo^2^)+(0.0976P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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Pb3 Pb 1.26241(11) 0.28697(5) 0.65431(4) 0.0216(2) Uani 1 1 d . . .
Pb4 Pb 2.05085(11) 0.33564(5) 0.84391(4) 0.0225(2) Uani 1 1 d . . .
Pb5 Pb 1.89448(12) 0.72443(7) 0.60052(5) 0.0316(2) Uani 1 1 d . . .
Pb6 Pb 1.74027(11) 0.62602(5) 0.78361(4) 0.0217(2) Uani 1 1 d . . .
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B4 B 1.690(3) 0.3617(15) 0.7415(11) 0.018(4) Uani 1 1 d U . .
B5 B 1.919(4) 0.4867(15) 0.6735(12) 0.022(4) Uani 1 1 d . . .
B6 B 2.204(3) 0.5969(15) 0.7309(11) 0.016(4) Uani 1 1 d . . .
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O14 O 2.105(2) 0.6353(11) 0.7887(8) 0.029(3) Uani 1 1 d . . .
O15 O 2.383(2) 0.6384(11) 0.7074(8) 0.027(3) Uani 1 1 d . . .
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Pb3 0.0307(4) 0.0155(4) 0.0191(4) -0.0014(2) 0.0045(3) 0.0009(3)
Pb4 0.0292(4) 0.0189(4) 0.0196(4) 0.0020(2) 0.0022(3) -0.0027(3)
Pb5 0.0279(4) 0.0332(5) 0.0339(5) 0.0120(3) 0.0049(3) -0.0011(3)
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B2 0.025(11) 0.026(12) 0.024(11) 0.014(9) -0.010(9) -0.013(9)
B3 0.026(11) 0.052(16) 0.010(9) -0.003(9) 0.010(8) -0.016(11)
B4 0.025(8) 0.011(7) 0.019(7) 0.006(6) 0.010(6) 0.007(6)
B5 0.034(12) 0.007(9) 0.027(11) 0.000(8) 0.017(9) 0.006(8)
B6 0.019(9) 0.014(9) 0.015(9) 0.003(7) 0.002(7) 0.003(8)
OW 0.111(12) 0.098(12) 0.093(12) 0.000(9) 0.012(9) 0.003(9)
O1 0.036(8) 0.009(6) 0.018(6) 0.001(5) 0.002(5) -0.010(5)
O2 0.026(6) 0.010(5) 0.024(6) -0.006(4) -0.004(5) 0.005(5)
O3 0.035(8) 0.013(6) 0.019(6) 0.000(5) 0.000(5) 0.003(6)
O4 0.026(6) 0.006(5) 0.014(6) -0.001(4) -0.002(5) -0.002(5)
O5 0.036(8) 0.027(8) 0.038(8) -0.010(6) -0.004(7) -0.005(7)
O6 0.034(8) 0.024(8) 0.019(7) 0.001(5) 0.003(6) 0.002(6)
O7 0.038(8) 0.028(8) 0.012(6) 0.005(5) 0.001(6) -0.011(6)
O8 0.031(7) 0.010(6) 0.027(7) -0.007(5) 0.010(6) -0.008(5)
O9 0.028(7) 0.026(7) 0.021(7) -0.005(5) 0.002(5) 0.009(6)
O10 0.030(7) 0.007(6) 0.015(6) 0.002(4) 0.002(5) 0.006(5)
O11 0.040(8) 0.009(6) 0.014(6) 0.001(5) -0.005(5) -0.006(6)
O12 0.031(7) 0.009(6) 0.022(6) -0.007(5) -0.001(5) 0.003(5)
O13 0.036(8) 0.018(7) 0.021(7) -0.006(5) 0.001(6) 0.000(6)
O14 0.037(8) 0.024(7) 0.027(7) -0.018(6) 0.003(6) 0.009(6)
O15 0.029(7) 0.023(7) 0.029(7) -0.013(6) 0.004(6) -0.010(6)
O16 0.044(8) 0.013(6) 0.023(7) -0.002(5) 0.010(6) 0.010(6)

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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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Pb1 O12 2.347(13) 3_866 ?
Pb1 O4 2.733(12) . ?
Pb1 Pb5 3.6556(11) 3_866 ?
Pb2 O5 2.200(16) 3_956 ?
Pb2 O16 2.277(13) 2_846 ?
Pb2 O3 2.407(13) 3_856 ?
Pb2 O5 2.617(14) . ?
Pb2 Pb2 3.6707(15) 3_856 ?
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Pb3 O3 2.197(13) . ?
Pb3 O14 2.408(14) 2_846 ?
Pb3 O7 2.442(15) . ?
Pb3 O6 2.751(15) 1_455 ?
Pb4 O10 2.299(13) . ?
Pb4 O1 2.349(13) 4_666 ?
Pb4 O16 2.396(14) . ?
Pb4 O11 2.550(12) . ?
Pb4 Pb5 3.4933(12) 2_846 ?
Pb5 O1 2.211(14) 3_866 ?
Pb5 O10 2.406(12) 2_856 ?
Pb5 O12 2.413(13) . ?
Pb5 O16 2.695(14) 2_856 ?
Pb5 OW 2.72(3) . ?
Pb5 Pb4 3.4933(12) 2_856 ?
Pb5 Pb1 3.6556(11) 3_866 ?
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Pb6 O10 2.315(12) 2_856 ?
Pb6 O14 2.404(16) . ?
Pb6 O15 2.654(15) 1_455 ?
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B1 O1 1.48(2) . ?
B1 O3 1.49(3) . ?
B1 O2 1.49(2) . ?
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B2 O2 1.37(2) . ?
B2 O6 1.41(3) . ?
B3 O4 1.45(3) . ?
B3 O7 1.45(2) . ?
B3 O8 1.50(3) . ?
B3 O6 1.51(3) . ?
B4 O11 1.42(3) . ?
B4 O7 1.49(2) . ?
B4 O10 1.49(2) . ?
B4 O9 1.51(2) . ?
B5 O8 1.44(2) . ?
B5 O13 1.46(3) . ?
B5 O12 1.50(2) . ?
B5 O11 1.51(2) . ?
B6 O14 1.36(2) . ?
B6 O13 1.37(2) . ?
B6 O15 1.39(2) . ?
O1 Pb5 2.211(14) 3_866 ?
O1 Pb4 2.349(13) 4_565 ?
O3 Pb2 2.407(13) 3_856 ?
O5 Pb2 2.200(16) 3_956 ?
O6 Pb3 2.751(15) 1_655 ?
O10 Pb6 2.315(12) 2_846 ?
O10 Pb5 2.406(12) 2_846 ?
O12 Pb1 2.347(13) 3_866 ?
O14 Pb3 2.408(14) 2_856 ?
O15 Pb1 2.343(14) 3_966 ?
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O16 Pb2 2.277(13) 2_856 ?
O16 Pb5 2.695(14) 2_846 ?

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O4 Pb1 Pb5 78.5(3) . 3_866 ?
O5 Pb2 O16 92.1(6) 3_956 2_846 ?
O5 Pb2 O3 86.5(5) 3_956 3_856 ?
O16 Pb2 O3 78.7(4) 2_846 3_856 ?
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O16 Pb2 O5 76.7(5) 2_846 . ?
O3 Pb2 O5 144.5(5) 3_856 . ?
O5 Pb2 Pb2 155.3(4) 3_956 3_856 ?
O16 Pb2 Pb2 71.0(4) 2_846 3_856 ?
O3 Pb2 Pb2 106.8(3) 3_856 3_856 ?
O5 Pb2 Pb2 88.9(4) . 3_856 ?
O3 Pb3 O14 91.6(5) . 2_846 ?
O3 Pb3 O7 85.0(5) . . ?
O14 Pb3 O7 80.8(5) 2_846 . ?
O3 Pb3 O6 77.5(5) . 1_455 ?
O14 Pb3 O6 107.7(5) 2_846 1_455 ?
O7 Pb3 O6 160.7(4) . 1_455 ?
O10 Pb4 O1 74.0(5) . 4_666 ?
O10 Pb4 O16 75.3(5) . . ?
O1 Pb4 O16 71.8(4) 4_666 . ?
O10 Pb4 O11 58.6(4) . . ?
O1 Pb4 O11 128.9(5) 4_666 . ?
O16 Pb4 O11 78.3(5) . . ?
O10 Pb4 Pb5 43.2(3) . 2_846 ?
O1 Pb4 Pb5 38.6(3) 4_666 2_846 ?
O16 Pb4 Pb5 50.4(3) . 2_846 ?
O11 Pb4 Pb5 90.7(3) . 2_846 ?
O1 Pb5 O10 74.5(4) 3_866 2_856 ?
O1 Pb5 O12 73.0(4) 3_866 . ?
O10 Pb5 O12 70.5(4) 2_856 . ?
O1 Pb5 O16 68.3(4) 3_866 2_856 ?
O10 Pb5 O16 68.2(4) 2_856 2_856 ?
O12 Pb5 O16 129.1(4) . 2_856 ?
O1 Pb5 OW 78.5(8) 3_866 . ?
O10 Pb5 OW 135.3(8) 2_856 . ?
O12 Pb5 OW 67.9(7) . . ?
O16 Pb5 OW 131.2(8) 2_856 . ?
O1 Pb5 Pb4 41.5(3) 3_866 2_856 ?
O10 Pb5 Pb4 40.9(3) 2_856 2_856 ?
O12 Pb5 Pb4 85.9(3) . 2_856 ?
O16 Pb5 Pb4 43.2(3) 2_856 2_856 ?
OW Pb5 Pb4 119.7(7) . 2_856 ?
O1 Pb5 Pb1 36.5(3) 3_866 3_866 ?
O10 Pb5 Pb1 78.8(3) 2_856 3_866 ?
O12 Pb5 Pb1 39.2(3) . 3_866 ?
O16 Pb5 Pb1 103.6(3) 2_856 3_866 ?
OW Pb5 Pb1 58.7(7) . 3_866 ?
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O5 B2 O6 122.4(18) . . ?
O2 B2 O6 120(2) . . ?
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B1 O3 Pb3 122.5(11) . . ?
B1 O3 Pb2 111.3(11) . 3_856 ?
Pb3 O3 Pb2 109.7(5) . 3_856 ?
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B2 O5 Pb2 136.9(13) . 3_956 ?
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B2 O6 Pb3 126.3(13) . 1_655 ?
B3 O6 Pb3 109.6(11) . 1_655 ?
B3 O7 B4 124.7(16) . . ?
B3 O7 Pb3 123.2(12) . . ?
B4 O7 Pb3 111.6(11) . . ?
B5 O8 B3 126.3(15) . . ?
B4 O10 Pb4 99.1(11) . . ?
B4 O10 Pb6 113.6(11) . 2_846 ?
Pb4 O10 Pb6 121.4(5) . 2_846 ?
B4 O10 Pb5 122.5(10) . 2_846 ?
Pb4 O10 Pb5 95.9(4) . 2_846 ?
Pb6 O10 Pb5 104.4(5) 2_846 2_846 ?
B4 O11 B5 125.5(15) . . ?
B4 O11 Pb4 90.6(10) . . ?
B5 O11 Pb4 130.7(12) . . ?
B5 O12 Pb6 103.2(10) . . ?
B5 O12 Pb1 116.9(11) . 3_866 ?
Pb6 O12 Pb1 109.8(5) . 3_866 ?
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B5 O12 Pb5 120.8(11) . . ?
Pb6 O12 Pb5 105.1(5) . . ?
Pb1 O12 Pb5 100.3(5) 3_866 . ?
B6 O13 B5 128.9(15) . . ?
B6 O14 Pb6 118.7(12) . . ?
B6 O14 Pb3 117.3(13) . 2_856 ?
Pb6 O14 Pb3 113.4(5) . 2_856 ?
B6 O15 Pb1 107.2(11) . 3_966 ?
B6 O15 Pb6 124.3(12) . 1_655 ?
Pb1 O15 Pb6 98.4(5) 3_966 1_655 ?
Pb2 O16 Pb4 131.2(7) 2_856 . ?
Pb2 O16 Pb5 104.1(5) 2_856 2_846 ?
Pb4 O16 Pb5 86.4(4) . 2_846 ?

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_refine_diff_density_rms    0.798
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