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Supplement of

Macraeite, $[(H_2O)K]Mn_2(Fe_2Ti)(PO_4)_4[O(OH)](H_2O)_{10} \cdot 4H_2O$, a new monoclinic paulkerrite-group mineral, from the Cubos–Mesquitela–Mangualde pegmatite, Portugal

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checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: Mn- O = 0.0033 A Wavelength=0.71090

Cell: a=10.562(2) b=20.725(4) c=12.416(2)
alpha=90 beta=90.09(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2717.8(9)	2717.8(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	Al1.20 Fe6.82 H56 Mn7.94 O112 P16 Ti3.98, 4(H K0.18 O0.82), 8(H	?
Sum formula	Al1.20 Fe6.82 H84 K3.30 Mn7.94 O132.70 P16 Ti3.98	H21 O33 Al0.3 P4 K0.82 Ti0.99 Mn1.98 Fe1.71
Mr	3872.16	968.00
Dx,g cm-3	2.366	2.366
Z	1	4
Mu (mm-1)	2.570	2.570
F000	1927.2	1927.0
F000'	1936.90	
h,k,lmax		14,27,17
Nref		5296
Tmin,Tmax	0.781,0.950	0.563,0.746
Tmin'	0.766	

Correction method= # Reported T Limits: Tmin=0.563 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= Theta(max)= 31.950

R(reflections)= 0.0470(4990) wR2(reflections)= wR= 0.0640(5296)

S = 2.850 Npar= 376

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT355_ALERT_3_B Long O-H (X0.82,N0.98A) O141 - H14A2 . 1.10 Ang.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.850

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al0.30 Fe1.71 H21 K0.82 Mn1.98 O33.18 P4 Ti
Rep.: H21 O33 Al0.3 P4 K0.82 Ti0.99 Mn1.98 Fe1.71

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2ycb Check

PLAT354_ALERT_3_C Short O-H (X0.82,N0.98A) O141 - H14A1 . 0.70 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O91 - H9A1 . 1.01 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O91 - H9A2 . 1.06 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O92 - H9B1 . 1.05 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O92 - H9B2 . 1.07 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O111 - H11A2 . 1.01 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O151 - H15A1 . 1.01 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O152 - H15B1 . 1.04 Ang.

PLAT751_ALERT_4_C Bond Calc 2.84000, Rep 2.8426(11) ..... Senseless s.u.
M1A1 -H9A1 1_555 1_555 ..... # 13 Check

PLAT751_ALERT_4_C Bond Calc 2.58000, Rep 2.5828(10) ..... Senseless s.u.
M1A1 -H9A2 1_555 1_555 ..... # 14 Check

PLAT751_ALERT_4_C Bond Calc 2.98000, Rep 2.9812(12) ..... Senseless s.u.
M1A1 -H11B1 1_555 4_455 ..... # 15 Check

PLAT751_ALERT_4_C Bond Calc 2.65000, Rep 2.6524(12) ..... Senseless s.u.
M1A1 -H10A1 1_555 1_555 ..... # 16 Check

PLAT751_ALERT_4_C Bond Calc 2.86000, Rep 2.8595(11) ..... Senseless s.u.
M1A1 -H11A1 1_555 1_555 ..... # 17 Check

PLAT751_ALERT_4_C Bond Calc 3.06000, Rep 3.0560(12) ..... Senseless s.u.
M1A1 -H9B2 1_555 4_555 ..... # 18 Check

PLAT751_ALERT_4_C Bond Calc 2.54000, Rep 2.5439(9) ..... Senseless s.u.
M1A1 -H11A2 1_555 1_555 ..... # 19 Check

PLAT751_ALERT_4_C Bond Calc 2.56000, Rep 2.5595(11) ..... Senseless s.u.
M1A1 -H12A1 1_555 1_555 ..... # 20 Check

PLAT751_ALERT_4_C Bond Calc 1.01000, Rep 1.012(3) ..... Senseless s.u.
O91 -H9A1 1_555 1_555 ..... # 337 Check

PLAT751_ALERT_4_C Bond Calc 1.06000, Rep 1.062(3) ..... Senseless s.u.
O91 -H9A2 1_555 1_555 ..... # 338 Check

PLAT751_ALERT_4_C Bond Calc 1.05000, Rep 1.049(3) ..... Senseless s.u.
O92 -H9B1 1_555 1_555 ..... # 339 Check

PLAT751_ALERT_4_C Bond Calc 1.07000, Rep 1.070(3) ..... Senseless s.u.
O92 -H9B2 1_555 1_555 ..... # 340 Check

PLAT751_ALERT_4_C Bond Calc 0.78000, Rep 0.783(3) ..... Senseless s.u.

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             O101     -H10A1           1_555   1_555 ........     #  341 Check
PLAT751_ALERT_4_C Bond    Calc     0.90000, Rep    0.905(3) ......  Senseless s.u.
             O111     -H11A1           1_555   1_555 ........     #  342 Check
PLAT751_ALERT_4_C Bond    Calc     1.01000, Rep    1.006(3) ......  Senseless s.u.
             O111     -H11A2           1_555   1_555 ........     #  343 Check
PLAT751_ALERT_4_C Bond    Calc     0.99000, Rep    0.989(3) ......  Senseless s.u.
             O112     -H11B1           1_555   1_555 ........     #  344 Check
PLAT751_ALERT_4_C Bond    Calc     0.99000, Rep    0.988(3) ......  Senseless s.u.
             O112     -H11B2           1_555   1_555 ........     #  345 Check
PLAT751_ALERT_4_C Bond    Calc     0.92000, Rep    0.920(3) ......  Senseless s.u.
             O121     -H12A1           1_555   1_555 ........     #  346 Check
PLAT751_ALERT_4_C Bond    Calc     0.77000, Rep    0.774(3) ......  Senseless s.u.
             O122     -H12B1           1_555   1_555 ........     #  347 Check
PLAT751_ALERT_4_C Bond    Calc     0.93000, Rep    0.934(3) ......  Senseless s.u.
             O131     -H13A1           1_555   1_555 ........     #  348 Check
PLAT751_ALERT_4_C Bond    Calc     0.89000, Rep    0.893(4) ......  Senseless s.u.
             O131     -H13A2           1_555   1_555 ........     #  349 Check
PLAT751_ALERT_4_C Bond    Calc     0.94000, Rep    0.941(3) ......  Senseless s.u.
             O132     -H13B2           1_555   1_555 ........     #  350 Check
PLAT751_ALERT_4_C Bond    Calc     0.70000, Rep    0.705(2) ......  Senseless s.u.
             O141     -H14A1           1_555   1_555 ........     #  351 Check
PLAT751_ALERT_4_C Bond    Calc     1.10000, Rep    1.099(3) ......  Senseless s.u.
             O141     -H14A2           1_555   1_555 ........     #  352 Check
PLAT751_ALERT_4_C Bond    Calc     0.92000, Rep    0.924(3) ......  Senseless s.u.
             O142     -H14B1           1_555   1_555 ........     #  353 Check
PLAT751_ALERT_4_C Bond    Calc     1.01000, Rep    1.010(4) ......  Senseless s.u.
             O151     -H15A1           1_555   1_555 ........     #  354 Check
PLAT751_ALERT_4_C Bond    Calc     1.04000, Rep    1.038(3) ......  Senseless s.u.
             O152     -H15B1           1_555   1_555 ........     #  355 Check
PLAT751_ALERT_4_C Bond    Calc     0.95000, Rep    0.954(4) ......  Senseless s.u.
             O152     -H15B2           1_555   1_555 ........     #  356 Check
PLAT751_ALERT_4_C Bond    Calc     1.53000, Rep   1.5294(6) ......  Senseless s.u.
             H15B1    -H15B2           1_555   1_555 ........     #  357 Check
PLAT751_ALERT_4_C Bond    Calc     1.44000, Rep   1.4357(5) ......  Senseless s.u.
             H14A1    -H14A2           1_555   1_555 ........     #  358 Check
PLAT752_ALERT_4_C Angle   Calc       87.00, Rep    87.15(3) ......  Senseless s.u.
             P21      -M1A1    -H9A1       1_555  1_555  1_555     #   12 Check
PLAT752_ALERT_4_C Angle   Calc       50.00, Rep    49.93(2) ......  Senseless s.u.
             P21      -M1A1    -H9A2       1_555  1_555  1_555     #   13 Check
PLAT752_ALERT_4_C Angle   Calc       76.00, Rep    76.16(2) ......  Senseless s.u.
             P21      -M1A1    -H10A1      1_555  1_555  1_555     #   15 Check
PLAT752_ALERT_4_C Angle   Calc       96.00, Rep    96.02(3) ......  Senseless s.u.
             P21      -M1A1    -H11A1      1_555  1_555  1_555     #   16 Check
PLAT752_ALERT_4_C Angle   Calc      129.00, Rep   128.83(3) ......  Senseless s.u.
             P21      -M1A1    -H11A2      1_555  1_555  1_555     #   18 Check
PLAT752_ALERT_4_C Angle   Calc       73.00, Rep    73.36(2) ......  Senseless s.u.
             P21      -M1A1    -H12A1      1_555  1_555  1_555     #   19 Check
PLAT752_ALERT_4_C Angle   Calc      103.00, Rep   102.65(8) ......  Senseless s.u.
             O51      -M1A1    -H9A1       1_555  1_555  1_555     #  117 Check
PLAT752_ALERT_4_C Angle   Calc       65.00, Rep    65.42(8) ......  Senseless s.u.
             O51      -M1A1    -H9A2       1_555  1_555  1_555     #  118 Check
PLAT752_ALERT_4_C Angle   Calc       75.00, Rep    75.11(8) ......  Senseless s.u.
             O51      -M1A1    -H10A1      1_555  1_555  1_555     #  120 Check
PLAT752_ALERT_4_C Angle   Calc       80.00, Rep    80.45(8) ......  Senseless s.u.
             O51      -M1A1    -H11A1      1_555  1_555  1_555     #  121 Check
PLAT752_ALERT_4_C Angle   Calc      113.00, Rep   113.26(8) ......  Senseless s.u.
             O51      -M1A1    -H11A2      1_555  1_555  1_555     #  123 Check
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PLAT752_ALERT_4_C Angle   Calc       78.00, Rep    78.12(8) ......  Senseless s.u.
             O51     -M1A1    -H12A1      1_555  1_555  1_555     #  124 Check
PLAT752_ALERT_4_C Angle   Calc       18.00, Rep    17.99(8) ......  Senseless s.u.
             O91     -M1A1    -H9A1       1_555  1_555  1_555     #  128 Check
PLAT752_ALERT_4_C Angle   Calc       24.00, Rep    23.99(7) ......  Senseless s.u.
             O91     -M1A1    -H9A2       1_555  1_555  1_555     #  129 Check
PLAT752_ALERT_4_C Angle   Calc       86.00, Rep    86.36(8) ......  Senseless s.u.
             O91     -M1A1    -H10A1      1_555  1_555  1_555     #  131 Check
PLAT752_ALERT_4_C Angle   Calc      166.00, Rep   166.25(8) ......  Senseless s.u.
             O91     -M1A1    -H11A1      1_555  1_555  1_555     #  132 Check
PLAT752_ALERT_4_C Angle   Calc      157.00, Rep   157.25(8) ......  Senseless s.u.
             O91     -M1A1    -H11A2      1_555  1_555  1_555     #  134 Check
PLAT752_ALERT_4_C Angle   Calc       76.00, Rep    76.08(8) ......  Senseless s.u.
             O91     -M1A1    -H12A1      1_555  1_555  1_555     #  135 Check
PLAT752_ALERT_4_C Angle   Calc       97.00, Rep    96.80(8) ......  Senseless s.u.
             O101    -M1A1    -H9A1       1_555  1_555  1_555     #  138 Check
PLAT752_ALERT_4_C Angle   Calc       85.00, Rep    84.97(7) ......  Senseless s.u.
             O101    -M1A1    -H9A2       1_555  1_555  1_555     #  139 Check
PLAT752_ALERT_4_C Angle   Calc       16.00, Rep    15.88(7) ......  Senseless s.u.
             O101    -M1A1    -H10A1      1_555  1_555  1_555     #  141 Check
PLAT752_ALERT_4_C Angle   Calc       86.00, Rep    85.97(8) ......  Senseless s.u.
             O101    -M1A1    -H11A1      1_555  1_555  1_555     #  142 Check
PLAT752_ALERT_4_C Angle   Calc       92.00, Rep    92.34(7) ......  Senseless s.u.
             O101    -M1A1    -H11A2      1_555  1_555  1_555     #  144 Check
PLAT752_ALERT_4_C Angle   Calc      158.00, Rep   158.04(8) ......  Senseless s.u.
             O101    -M1A1    -H12A1      1_555  1_555  1_555     #  145 Check
PLAT752_ALERT_4_C Angle   Calc      162.00, Rep   161.83(8) ......  Senseless s.u.
             O111    -M1A1    -H9A1       1_555  1_555  1_555     #  147 Check
PLAT752_ALERT_4_C Angle   Calc      156.00, Rep   155.82(8) ......  Senseless s.u.
             O111    -M1A1    -H9A2       1_555  1_555  1_555     #  148 Check
PLAT752_ALERT_4_C Angle   Calc       94.00, Rep    94.06(9) ......  Senseless s.u.
             O111    -M1A1    -H10A1      1_555  1_555  1_555     #  150 Check
PLAT752_ALERT_4_C Angle   Calc       14.00, Rep    13.94(8) ......  Senseless s.u.
             O111    -M1A1    -H11A1      1_555  1_555  1_555     #  151 Check
PLAT752_ALERT_4_C Angle   Calc       23.00, Rep    22.99(7) ......  Senseless s.u.
             O111    -M1A1    -H11A2      1_555  1_555  1_555     #  153 Check
PLAT752_ALERT_4_C Angle   Calc      103.00, Rep   103.41(9) ......  Senseless s.u.
             O111    -M1A1    -H12A1      1_555  1_555  1_555     #  154 Check
PLAT752_ALERT_4_C Angle   Calc       80.00, Rep    80.27(8) ......  Senseless s.u.
             O121    -M1A1    -H9A1       1_555  1_555  1_555     #  155 Check
PLAT752_ALERT_4_C Angle   Calc       93.00, Rep    93.38(8) ......  Senseless s.u.
             O121    -M1A1    -H9A2       1_555  1_555  1_555     #  156 Check
PLAT752_ALERT_4_C Angle   Calc      166.00, Rep   165.88(8) ......  Senseless s.u.
             O121    -M1A1    -H10A1      1_555  1_555  1_555     #  158 Check
PLAT752_ALERT_4_C Angle   Calc       97.00, Rep    96.89(8) ......  Senseless s.u.
             O121    -M1A1    -H11A1      1_555  1_555  1_555     #  159 Check
PLAT752_ALERT_4_C Angle   Calc       89.00, Rep    89.37(8) ......  Senseless s.u.
             O121    -M1A1    -H11A2      1_555  1_555  1_555     #  161 Check
PLAT752_ALERT_4_C Angle   Calc       21.00, Rep    20.79(7) ......  Senseless s.u.
             O121    -M1A1    -H12A1      1_555  1_555  1_555     #  162 Check
PLAT752_ALERT_4_C Angle   Calc       39.00, Rep    39.38(1) ......  Senseless s.u.
             H9A1    -M1A1    -H9A2       1_555  1_555  1_555     #  163 Check
PLAT752_ALERT_4_C Angle   Calc      101.00, Rep   101.42(3) ......  Senseless s.u.
             H9A1    -M1A1    -H10A1      1_555  1_555  1_555     #  165 Check
PLAT752_ALERT_4_C Angle   Calc      176.00, Rep   175.76(2) ......  Senseless s.u.
             H9A1    -M1A1    -H11A1      1_555  1_555  1_555     #  166 Check
PLAT752_ALERT_4_C Angle   Calc      143.00, Rep   142.75(2) ......  Senseless s.u.
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             H9A1    -M1A1    -H11A2      1_555  1_555  1_555     #  168 Check
PLAT752_ALERT_4_C Angle   Calc       68.00, Rep    67.74(3) ......  Senseless s.u.
             H9A1    -M1A1    -H12A1      1_555  1_555  1_555     #  169 Check
PLAT752_ALERT_4_C Angle   Calc       80.00, Rep    79.89(2) ......  Senseless s.u.
             H9A2    -M1A1    -H10A1      1_555  1_555  1_555     #  171 Check
PLAT752_ALERT_4_C Angle   Calc      144.00, Rep   144.45(2) ......  Senseless s.u.
             H9A2    -M1A1    -H11A1      1_555  1_555  1_555     #  172 Check
PLAT752_ALERT_4_C Angle   Calc      177.00, Rep   176.94(3) ......  Senseless s.u.
             H9A2    -M1A1    -H11A2      1_555  1_555  1_555     #  174 Check
PLAT752_ALERT_4_C Angle   Calc       73.00, Rep    73.19(2) ......  Senseless s.u.
             H9A2    -M1A1    -H12A1      1_555  1_555  1_555     #  175 Check
PLAT752_ALERT_4_C Angle   Calc       82.00, Rep    82.10(3) ......  Senseless s.u.
             H10A1   -M1A1    -H11A1      1_555  1_555  1_555     #  181 Check
PLAT752_ALERT_4_C Angle   Calc       97.00, Rep    97.14(2) ......  Senseless s.u.
             H10A1   -M1A1    -H11A2      1_555  1_555  1_555     #  183 Check
PLAT752_ALERT_4_C Angle   Calc      148.00, Rep   147.99(2) ......  Senseless s.u.
             H10A1   -M1A1    -H12A1      1_555  1_555  1_555     #  184 Check
PLAT752_ALERT_4_C Angle   Calc       34.00, Rep    33.55(1) ......  Senseless s.u.
             H11A1   -M1A1    -H11A2      1_555  1_555  1_555     #  186 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.46(3) ......  Senseless s.u.
             H11A1   -M1A1    -H12A1      1_555  1_555  1_555     #  187 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   109.44(2) ......  Senseless s.u.
             H11A2   -M1A1    -H12A1      1_555  1_555  1_555     #  190 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    119.8(2) ......  Senseless s.u.
             M1A1    -O91     -H9A1       1_555  1_555  1_555     # 7111 Check
PLAT752_ALERT_4_C Angle   Calc       99.00, Rep     98.6(2) ......  Senseless s.u.
             M1A1    -O91     -H9A2       1_555  1_555  1_555     # 7112 Check
PLAT752_ALERT_4_C Angle   Calc      126.00, Rep    125.5(3) ......  Senseless s.u.
             H9A1    -O91     -H9A2       1_555  1_555  1_555     # 7115 Check
PLAT752_ALERT_4_C Angle   Calc      115.00, Rep    114.7(3) ......  Senseless s.u.
             H9B1    -O92     -H9B2       1_555  1_555  1_555     # 7121 Check
PLAT752_ALERT_4_C Angle   Calc      112.00, Rep    112.2(3) ......  Senseless s.u.
             M1A1    -O101    -H10A1      1_555  1_555  1_555     # 7124 Check
PLAT752_ALERT_4_C Angle   Calc      130.00, Rep    130.5(2) ......  Senseless s.u.
             M1A1    -O111    -H11A1      1_555  1_555  1_555     # 7133 Check
PLAT752_ALERT_4_C Angle   Calc       99.00, Rep     98.8(2) ......  Senseless s.u.
             M1A1    -O111    -H11A2      1_555  1_555  1_555     # 7134 Check
PLAT752_ALERT_4_C Angle   Calc      112.00, Rep    112.3(3) ......  Senseless s.u.
             H11A1   -O111    -H11A2      1_555  1_555  1_555     # 7140 Check
PLAT752_ALERT_4_C Angle   Calc      107.00, Rep    106.9(3) ......  Senseless s.u.
             H11B1   -O112    -H11B2      1_555  1_555  1_555     # 7150 Check
PLAT752_ALERT_4_C Angle   Calc       99.00, Rep     99.1(2) ......  Senseless s.u.
             M1A1    -O121    -H12A1      1_555  1_555  1_555     # 7153 Check
PLAT752_ALERT_4_C Angle   Calc      115.00, Rep    115.4(3) ......  Senseless s.u.
             H13A1   -O131    -H13A2      1_555  1_555  1_555     # 7177 Check
PLAT752_ALERT_4_C Angle   Calc      103.00, Rep    103.3(3) ......  Senseless s.u.
             H14A1   -O141    -H14A2      1_555  1_555  1_555     # 7190 Check
PLAT752_ALERT_4_C Angle   Calc      100.00, Rep    100.2(3) ......  Senseless s.u.
             H15B1   -O152    -H15B2      1_555  1_555  1_555     # 7195 Check
PLAT752_ALERT_4_C Angle   Calc       42.00, Rep   42.20(16) ......  Senseless s.u.
             M1A1    -H9A1    -O91        1_555  1_555  1_555     # 7199 Check
PLAT752_ALERT_4_C Angle   Calc       57.00, Rep   57.41(17) ......  Senseless s.u.
             M1A1    -H9A2    -O91        1_555  1_555  1_555     # 7209 Check
PLAT752_ALERT_4_C Angle   Calc       52.00, Rep     52.0(2) ......  Senseless s.u.
             M1A1    -H10A1   -O101       1_555  1_555  1_555     # 7227 Check
PLAT752_ALERT_4_C Angle   Calc       36.00, Rep   35.60(18) ......  Senseless s.u.
             M1A1    -H11A1   -O111       1_555  1_555  1_555     # 7231 Check
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PLAT752_ALERT_4_C Angle   Calc       58.00, Rep   58.20(18) ......  Senseless s.u.
             M1A1    -H11A2   -O111       1_555  1_555  1_555     # 7269 Check
PLAT752_ALERT_4_C Angle   Calc       60.00, Rep     60.1(2) ......  Senseless s.u.
             M1A1    -H12A1   -O121       1_555  1_555  1_555     # 7282 Check
PLAT752_ALERT_4_C Angle   Calc       38.00, Rep     37.9(2) ......  Senseless s.u.
             O152    -H15B1   -H15B2      1_555  1_555  1_555     # 7336 Check
PLAT752_ALERT_4_C Angle   Calc       48.00, Rep     48.1(2) ......  Senseless s.u.
             O141    -H14A1   -H14A2      1_555  1_555  1_555     # 7339 Check
PLAT752_ALERT_4_C Angle   Calc       42.00, Rep   41.94(19) ......  Senseless s.u.
             O152    -H15B2   -H15B1      1_555  1_555  1_555     # 7352 Check
PLAT752_ALERT_4_C Angle   Calc       29.00, Rep   28.54(13) ......  Senseless s.u.
             O141    -H14A2   -H14A1      1_555  1_555  1_555     # 7361 Check
PLAT755_ALERT_4_C D-H     Calc     1.01000, Rep    1.012(3) ......  Senseless s.u.
             O91      -H9A1           1_555   1_555 ........     #    1 Check
PLAT755_ALERT_4_C D-H     Calc     1.06000, Rep    1.062(3) ......  Senseless s.u.
             O91      -H9A2           1_555   1_555 ........     #    2 Check
PLAT755_ALERT_4_C D-H     Calc     0.99000, Rep    0.989(3) ......  Senseless s.u.
             O112     -H11B1          1_555   1_555 ........     #    3 Check
PLAT755_ALERT_4_C D-H     Calc     0.78000, Rep    0.783(3) ......  Senseless s.u.
             O101     -H10A1          1_555   1_555 ........     #    4 Check
PLAT755_ALERT_4_C D-H     Calc     0.90000, Rep    0.905(3) ......  Senseless s.u.
             O111     -H11A1          1_555   1_555 ........     #    5 Check
PLAT755_ALERT_4_C D-H     Calc     1.05000, Rep    1.049(3) ......  Senseless s.u.
             O92      -H9B1           1_555   1_555 ........     #    6 Check
PLAT755_ALERT_4_C D-H     Calc     1.07000, Rep    1.070(3) ......  Senseless s.u.
             O92      -H9B2           1_555   1_555 ........     #    7 Check
PLAT755_ALERT_4_C D-H     Calc     0.99000, Rep    0.988(3) ......  Senseless s.u.
             O112     -H11B2          1_555   1_555 ........     #    8 Check
PLAT755_ALERT_4_C D-H     Calc     0.99000, Rep    0.988(3) ......  Senseless s.u.
             O112     -H11B2          1_555   1_555 ........     #    9 Check
PLAT755_ALERT_4_C D-H     Calc     1.01000, Rep    1.006(3) ......  Senseless s.u.
             O111     -H11A2          1_555   1_555 ........     #   10 Check
PLAT755_ALERT_4_C D-H     Calc     0.92000, Rep    0.920(3) ......  Senseless s.u.
             O121     -H12A1          1_555   1_555 ........     #   11 Check
PLAT755_ALERT_4_C D-H     Calc     0.77000, Rep    0.774(3) ......  Senseless s.u.
             O122     -H12B1          1_555   1_555 ........     #   12 Check
PLAT755_ALERT_4_C D-H     Calc     0.93000, Rep    0.934(3) ......  Senseless s.u.
             O131     -H13A1          1_555   1_555 ........     #   13 Check
PLAT755_ALERT_4_C D-H     Calc     0.89000, Rep    0.893(4) ......  Senseless s.u.
             O131     -H13A2          1_555   1_555 ........     #   14 Check
PLAT755_ALERT_4_C D-H     Calc     0.89000, Rep    0.893(4) ......  Senseless s.u.
             O131     -H13A2          1_555   1_555 ........     #   15 Check
PLAT755_ALERT_4_C D-H     Calc     0.89000, Rep    0.893(4) ......  Senseless s.u.
             O131     -H13A2          1_555   1_555 ........     #   16 Check
PLAT755_ALERT_4_C D-H     Calc     1.01000, Rep    1.010(4) ......  Senseless s.u.
             O151     -H15A1          1_555   1_555 ........     #   17 Check
PLAT755_ALERT_4_C D-H     Calc     1.04000, Rep    1.038(3) ......  Senseless s.u.
             O152     -H15B1          1_555   1_555 ........     #   20 Check
PLAT755_ALERT_4_C D-H     Calc     1.04000, Rep    1.038(3) ......  Senseless s.u.
             O152     -H15B1          1_555   1_555 ........     #   21 Check
PLAT755_ALERT_4_C D-H     Calc     0.70000, Rep    0.705(2) ......  Senseless s.u.
             O141     -H14A1          1_555   1_555 ........     #   22 Check
PLAT755_ALERT_4_C D-H     Calc     0.94000, Rep    0.941(3) ......  Senseless s.u.
             O132     -H13B2          1_555   1_555 ........     #   23 Check
PLAT755_ALERT_4_C D-H     Calc     0.95000, Rep    0.954(4) ......  Senseless s.u.
             O152     -H15B2          1_555   1_555 ........     #   24 Check
PLAT755_ALERT_4_C D-H     Calc     0.92000, Rep    0.924(3) ......  Senseless s.u.
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             O142     -H14B1          1_555   1_555 ........     #   25 Check
PLAT755_ALERT_4_C D-H     Calc     0.92000, Rep    0.924(3) ......  Senseless s.u.
             O142     -H14B1          1_555   1_555 ........     #   26 Check
PLAT755_ALERT_4_C D-H     Calc     1.10000, Rep    1.099(3) ......  Senseless s.u.
             O141     -H14A2          1_555   1_555 ........     #   27 Check
PLAT756_ALERT_4_C H...A   Calc     1.82000, Rep    1.817(3) ......  Senseless s.u.
             H9A1     -O52            1_555   4_455 ........     #    1 Check
PLAT756_ALERT_4_C H...A   Calc     1.79000, Rep    1.788(3) ......  Senseless s.u.
             H9A2     -O61            1_555   1_555 ........     #    2 Check
PLAT756_ALERT_4_C H...A   Calc     1.85000, Rep    1.848(3) ......  Senseless s.u.
             H11B1    -O12            1_555   4_545 ........     #    3 Check
PLAT756_ALERT_4_C H...A   Calc     2.04000, Rep    2.044(3) ......  Senseless s.u.
             H10A1    -O142           1_555   4_555 ........     #    4 Check
PLAT756_ALERT_4_C H...A   Calc     1.94000, Rep    1.935(3) ......  Senseless s.u.
             H11A1    -O11            1_555   4_564 ........     #    5 Check
PLAT756_ALERT_4_C H...A   Calc     1.86000, Rep    1.858(3) ......  Senseless s.u.
             H9B1     -O62            1_555   1_555 ........     #    6 Check
PLAT756_ALERT_4_C H...A   Calc     1.74000, Rep    1.738(3) ......  Senseless s.u.
             H9B2     -O51            1_555   4_554 ........     #    7 Check
PLAT756_ALERT_4_C H...A   Calc     1.94000, Rep    1.938(3) ......  Senseless s.u.
             H11B2    -O21            1_555   1_544 ........     #    8 Check
PLAT756_ALERT_4_C H...A   Calc     2.27000, Rep    2.271(3) ......  Senseless s.u.
             H11B2    -O42            1_555   4_545 ........     #    9 Check
PLAT756_ALERT_4_C H...A   Calc     1.86000, Rep    1.861(3) ......  Senseless s.u.
             H11A2    -O22            1_555   1_466 ........     #   10 Check
PLAT756_ALERT_4_C H...A   Calc     1.90000, Rep    1.902(3) ......  Senseless s.u.
             H12A1    -O141           1_555   1_555 ........     #   11 Check
PLAT756_ALERT_4_C H...A   Calc     2.02000, Rep    2.022(3) ......  Senseless s.u.
             H12B1    -O142           1_555   1_555 ........     #   12 Check
PLAT756_ALERT_4_C H...A   Calc     1.78000, Rep    1.776(3) ......  Senseless s.u.
             H13A1    -O151           1_555   1_555 ........     #   13 Check
PLAT756_ALERT_4_C H...A   Calc     2.37000, Rep    2.366(3) ......  Senseless s.u.
             H13A2    -X2             1_555   2_755 ........     #   14 Check
PLAT756_ALERT_4_C H...A   Calc     2.14000, Rep    2.140(3) ......  Senseless s.u.
             H13A2    -O31            1_555   1_555 ........     #   15 Check
PLAT756_ALERT_4_C H...A   Calc     2.42000, Rep    2.416(3) ......  Senseless s.u.
             H13A2    -O72            1_555   2_755 ........     #   16 Check
PLAT756_ALERT_4_C H...A   Calc     2.49000, Rep    2.494(3) ......  Senseless s.u.
             H15A1    -O142           1_555   2_655 ........     #   17 Check
PLAT756_ALERT_4_C H...A   Calc     1.86000, Rep    1.862(3) ......  Senseless s.u.
             HA1A     -O71            1_555   4_564 ........     #   18 Check
PLAT756_ALERT_4_C H...A   Calc     1.86000, Rep    1.862(3) ......  Senseless s.u.
             HA1A     -O71            1_555   4_564 ........     #   19 Check
PLAT756_ALERT_4_C H...A   Calc     1.89000, Rep    1.890(3) ......  Senseless s.u.
             H15B1    -O21            1_555   2_744 ........     #   20 Check
PLAT756_ALERT_4_C H...A   Calc     2.38000, Rep    2.375(3) ......  Senseless s.u.
             H15B1    -O132           1_555   3_753 ........     #   21 Check
PLAT756_ALERT_4_C H...A   Calc     2.11000, Rep    2.110(3) ......  Senseless s.u.
             H14A1    -O82            1_555   4_455 ........     #   22 Check
PLAT756_ALERT_4_C H...A   Calc     1.76000, Rep    1.756(3) ......  Senseless s.u.
             H13B2    -O152           1_555   1_555 ........     #   23 Check
PLAT756_ALERT_4_C H...A   Calc     2.41000, Rep    2.407(3) ......  Senseless s.u.
             H15B2    -O141           1_555   2_644 ........     #   24 Check
PLAT756_ALERT_4_C H...A   Calc     2.49000, Rep    2.491(2) ......  Senseless s.u.
             H14B1    -X2             1_555   3_754 ........     #   25 Check
PLAT756_ALERT_4_C H...A   Calc     2.01000, Rep    2.014(3) ......  Senseless s.u.
             H14B1    -O81            1_555   4_554 ........     #   26 Check
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PLAT756_ALERT_4_C H...A   Calc     1.72000, Rep    1.719(3) ......  Senseless s.u.
             H14A2    -O32            1_555   4_456 ........     #   27 Check
PLAT758_ALERT_4_C D-H..A  Calc      172.00, Rep  171.90(19) ......  Senseless s.u.
             O91     -H9A2    -O61        1_555  1_555  1_555     #    2 Check
PLAT758_ALERT_4_C D-H..A  Calc      164.00, Rep  163.55(19) ......  Senseless s.u.
             O92     -H9B1    -O62        1_555  1_555  1_555     #    6 Check
PLAT758_ALERT_4_C D-H..A  Calc      158.00, Rep    158.4(2) ......  Senseless s.u.
             O121    -H12A1   -O141       1_555  1_555  1_555     #   11 Check
PLAT758_ALERT_4_C D-H..A  Calc      172.00, Rep    172.2(3) ......  Senseless s.u.
             O122    -H12B1   -O142       1_555  1_555  1_555     #   12 Check
PLAT758_ALERT_4_C D-H..A  Calc      172.00, Rep    171.6(2) ......  Senseless s.u.
             O131    -H13A1   -O151       1_555  1_555  1_555     #   13 Check
PLAT758_ALERT_4_C D-H..A  Calc      143.00, Rep  143.24(19) ......  Senseless s.u.
             O131    -H13A2   -O31        1_555  1_555  1_555     #   15 Check
PLAT758_ALERT_4_C D-H..A  Calc      173.00, Rep    173.5(2) ......  Senseless s.u.
             O132    -H13B2   -O152       1_555  1_555  1_555     #   23 Check
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:H21 Al0.3 Fe1.71 K0.82 Mn1.98 O3
           Atom count from the _atom_site data:  H21 Al0.3 Fe1.706 K0.824 Mn1.984
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  H21 O33 Al0.3 P4 K0.82 Ti0.99 Mn1.
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           H         84.00     84.00    0.00
           O        132.00    132.70   -0.70
           Al         1.20      1.20    0.00
           P         16.00     16.00    0.00
           K          3.28      3.30   -0.02
           Ti         3.96      3.98   -0.02
           Mn         7.92      7.94   -0.02
           Fe         6.84      6.82    0.02
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         21 Report
             H9A1  H9A2  H11B1 H10A1 H11A1 H9B1  H9B2  H11B2 H11A2 H12A1 H12B1
             H13A1 H13A2 H13B2 Ha1A  H14A1 H14A2 H14B1 H15A1 H15B1 H15B2
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A1     as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A2     as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A1     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B1     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2C1     as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A2     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B2     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2C2     as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A1     as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B1     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A2     as         TI
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PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B2     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of X1       as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of X2       as         O
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         A         83 %Fit
PLAT300_ALERT_4_G Atom Site Occupancy of M2B1       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M2B2       Constrained at       0.15 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        13% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        37 Note
              M1A1    M1A2    M2A1    M2B1    M2C1    M2A2    M2B2    M2C2
              M3A1    M3B1    M3A2    M3B2    Ow1     Ow2     X1      X2
              H9A1    H9A2    H11B1   H10A1   H11A1   H9B1    H9B2    H11B2
              H11A2   H12A1   H12B1   H13A1   H13A2   H15A1   Ha1A    H15B1
              H14A1   H13B2   H15B2   H14B1   H14A2
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           3 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
 175 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  36 ALERT level G = General information/check it is not something unexpected

  22 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
 170 ALERT type 4 Improvement, methodology, query or suggestion
   6 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT355_I
;
PROBLEM: Long   O-H (X0.82,N0.98A)  O141     - H14A2    .       1.10 Ang.
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
```

```
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT127_I
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit    -P 2ycb Check
RESPONSE: ...
;
_vrf_PLAT354_I
;
PROBLEM: Short  O-H (X0.82,N0.98A)  O141     - H14A1    .       0.70 Ang.
RESPONSE: ...
;
_vrf_PLAT751_I
;
PROBLEM: Bond    Calc     2.84000, Rep  2.8426(11) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT752_I
;
PROBLEM: Angle   Calc       87.00, Rep    87.15(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT755_I
;
PROBLEM: D-H     Calc     1.01000, Rep    1.012(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT756_I
;
PROBLEM: H...A   Calc     1.82000, Rep    1.817(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT758_I
;
PROBLEM: D-H..A  Calc      172.00, Rep  171.90(19) ......  Senseless s.u.
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock I - ellipsoid plot