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:   P- O = 0.0023 A          Wavelength=0.71090

Cell:              a=10.440(5)      b=20.588(5)         c=12.234(2)
                   alpha=90         beta=90.38(1)       gamma=90
Temperature:       100 K
```

	Calculated	Reported
Volume	2629.5(15)	2629.5(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	Al7.35 Fe2.75 H80 K0.01 Mg1.06 Mn6.94 O115.83 P16 Ti1.90, 16(H2	?
Sum formula	Al7.35 Fe2.75 H112 K3.82 Mg1.06 Mn6.94 O131.86 P16 Ti1.90	H28 O32.958 Mg0.255 Al1.835 P4 K0.962 Ti0.482 Mn1.745 Fe0.683
Mr	3717.39	929.30
Dx,g cm-3	2.348	2.348
Z	1	4
Mu (mm-1)	1.934	1.884
F000	1874.5	1875.0
F000'	1882.45	
h,k,lmax	15,30,18	15,30,17
Nref	9214	7749
Tmin,Tmax	0.914,0.945	0.480,0.750
Tmin'	0.860	

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Correction method= # Reported T Limits: Tmin=0.480 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.841           Theta(max)= 32.120
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R(reflections)= 0.0595(5951)

wR2(reflections)=
wR= 0.0774(7749)

S = 2.130 Npar= 377

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

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PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem         a        100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem         b        100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New  Space Group       Pbca Check
              WARNING: Disordered Atoms Excluded from Analysis
              Check Model Parameter Symmetry for Reflection Data Support
PLAT355_ALERT_3_B Long   O-H (X0.82,N0.98A)  O13B     - H13B2    .       1.11 Ang.
PLAT416_ALERT_2_B Short Intra D-H..H-D       Ha1A     ..H12B1    .       1.64 Ang.
                                              x,1/2-y,1/2+z  =      4_555 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D       H12B2    ..H14B1    .       2.04 Ang.
                                             x,y,z  =      1_555 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D       H13B2    ..H15B1    .       2.09 Ang.
                                             x,y,z  =      1_555 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D       H13B2    ..H15B2    .       1.97 Ang.
                                             x,y,z  =      1_555 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O12B     --H12B1    .     Please Check
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Alert level C

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GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      2.130
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: Al1.84 Fe0.69 H28 K0.96 Mg0.27 Mn1.73 O32.96 P4 Ti0.48
             Rep.: H28 O32.958 Mg0.255 Al1.835 P4 K0.962 Ti0.482
                   Mn1.745 Fe0.683
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.67 %
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
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O9A      -H9A2      .      45.85 Degree
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O9A      - H9A1     .       1.04 Ang.
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O9B      - H9B2     .       1.06 Ang.
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O12B     - H12B2    .       1.03 Ang.
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O15A     - H15A2    .       1.07 Ang.
PLAT751_ALERT_4_C Bond    Calc     1.04000, Rep    1.043(3) ......  Senseless s.u.
             O9A      -H9A1           1_555   1_555 ........     #  280 Check
PLAT751_ALERT_4_C Bond    Calc     0.91000, Rep    0.912(2) ......  Senseless s.u.
             O9A      -H9A2           1_555   1_555 ........     #  281 Check
PLAT751_ALERT_4_C Bond    Calc     0.85000, Rep    0.851(3) ......  Senseless s.u.
             O9B      -H9B1           1_555   1_555 ........     #  282 Check
PLAT751_ALERT_4_C Bond    Calc     1.06000, Rep    1.056(2) ......  Senseless s.u.
             O9B      -H9B2           1_555   1_555 ........     #  283 Check
PLAT751_ALERT_4_C Bond    Calc     0.78000, Rep    0.781(2) ......  Senseless s.u.
             O10A     -H10A1          1_555   1_555 ........     #  284 Check
PLAT751_ALERT_4_C Bond    Calc     0.85000, Rep    0.847(2) ......  Senseless s.u.
             O10B     -H10B1          1_555   1_555 ........     #  285 Check
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PLAT751_ALERT_4_C Bond    Calc     0.77000, Rep    0.773(2) ......  Senseless s.u.
             O10B     -H10B2          1_555   1_555 ........     #  286 Check
PLAT751_ALERT_4_C Bond    Calc     0.84000, Rep    0.837(3) ......  Senseless s.u.
             O11A     -H11A1          1_555   1_555 ........     #  287 Check
PLAT751_ALERT_4_C Bond    Calc     0.92000, Rep    0.917(2) ......  Senseless s.u.
             O11A     -H11A2          1_555   1_555 ........     #  288 Check
PLAT751_ALERT_4_C Bond    Calc     0.79000, Rep    0.787(3) ......  Senseless s.u.
             O11B     -H11B1          1_555   1_555 ........     #  289 Check
PLAT751_ALERT_4_C Bond    Calc     0.86000, Rep    0.861(2) ......  Senseless s.u.
             O11B     -H11B2          1_555   1_555 ........     #  290 Check
PLAT751_ALERT_4_C Bond    Calc     0.84000, Rep    0.844(2) ......  Senseless s.u.
             O12A     -H12A1          1_555   1_555 ........     #  291 Check
PLAT751_ALERT_4_C Bond    Calc     0.93000, Rep    0.927(2) ......  Senseless s.u.
             O12B     -H12B1          1_555   1_555 ........     #  292 Check
PLAT751_ALERT_4_C Bond    Calc     1.03000, Rep    1.028(2) ......  Senseless s.u.
             O12B     -H12B2          1_555   1_555 ........     #  293 Check
PLAT751_ALERT_4_C Bond    Calc     0.90000, Rep    0.902(2) ......  Senseless s.u.
             O13A     -H13A1          1_555   1_555 ........     #  294 Check
PLAT751_ALERT_4_C Bond    Calc     0.83000, Rep    0.829(3) ......  Senseless s.u.
             O13A     -H13A2          1_555   1_555 ........     #  295 Check
PLAT751_ALERT_4_C Bond    Calc     0.90000, Rep    0.902(3) ......  Senseless s.u.
             O13B     -H13B1          1_555   1_555 ........     #  296 Check
PLAT751_ALERT_4_C Bond    Calc     1.11000, Rep    1.114(3) ......  Senseless s.u.
             O13B     -H13B2          1_555   1_555 ........     #  297 Check
PLAT751_ALERT_4_C Bond    Calc     0.81000, Rep    0.808(2) ......  Senseless s.u.
             O14A     -H14A1          1_555   1_555 ........     #  298 Check
PLAT751_ALERT_4_C Bond    Calc     0.74000, Rep    0.741(3) ......  Senseless s.u.
             O14A     -H14A2          1_555   1_555 ........     #  299 Check
PLAT751_ALERT_4_C Bond    Calc     0.77000, Rep    0.772(2) ......  Senseless s.u.
             O14B     -H14B1          1_555   1_555 ........     #  300 Check
PLAT751_ALERT_4_C Bond    Calc     0.86000, Rep    0.865(2) ......  Senseless s.u.
             O14B     -H14B2          1_555   1_555 ........     #  301 Check
PLAT751_ALERT_4_C Bond    Calc     0.97000, Rep    0.974(3) ......  Senseless s.u.
             O15A     -H15A1          1_555   1_555 ........     #  302 Check
PLAT751_ALERT_4_C Bond    Calc     1.07000, Rep    1.069(2) ......  Senseless s.u.
             O15A     -H15A2          1_555   1_555 ........     #  303 Check
PLAT751_ALERT_4_C Bond    Calc     0.85000, Rep    0.846(2) ......  Senseless s.u.
             O15B     -H15B1          1_555   1_555 ........     #  304 Check
PLAT751_ALERT_4_C Bond    Calc     0.85000, Rep    0.851(3) ......  Senseless s.u.
             O15B     -H15B2          1_555   1_555 ........     #  305 Check
PLAT751_ALERT_4_C Bond    Calc     1.33000, Rep   1.3315(9) ......  Senseless s.u.
             HA1A     -HA1B           1_555   1_555 ........     #  306 Check
PLAT751_ALERT_4_C Bond    Calc     1.33000, Rep   1.3319(9) ......  Senseless s.u.
             H10B1    -H10B2          1_555   1_555 ........     #  307 Check
PLAT751_ALERT_4_C Bond    Calc     1.35000, Rep   1.3487(7) ......  Senseless s.u.
             H11A1    -H11A2          1_555   1_555 ........     #  308 Check
PLAT751_ALERT_4_C Bond    Calc     1.24000, Rep   1.2405(7) ......  Senseless s.u.
             H11B1    -H11B2          1_555   1_555 ........     #  309 Check
PLAT751_ALERT_4_C Bond    Calc     1.31000, Rep   1.3111(9) ......  Senseless s.u.
             H13A1    -H13A2          1_555   1_555 ........     #  310 Check
PLAT751_ALERT_4_C Bond    Calc     1.20000, Rep   1.1965(4) ......  Senseless s.u.
             H14A1    -H14A2          1_555   1_555 ........     #  311 Check
PLAT751_ALERT_4_C Bond    Calc     1.30000, Rep   1.2957(4) ......  Senseless s.u.
             H14B1    -H14B2          1_555   1_555 ........     #  312 Check
PLAT752_ALERT_4_C Angle   Calc       99.00, Rep     99.3(2) ......  Senseless s.u.
             H9A1    -O9A     -H9A2       1_555  1_555  1_555     # 4685 Check
PLAT752_ALERT_4_C Angle   Calc       95.00, Rep     94.6(2) ......  Senseless s.u.
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             H9B1    -O9B     -H9B2       1_555  1_555  1_555     # 4695 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep    110.5(3) ......  Senseless s.u.
             H10B1   -O10B    -H10B2      1_555  1_555  1_555     # 4711 Check
PLAT752_ALERT_4_C Angle   Calc      100.00, Rep    100.4(2) ......  Senseless s.u.
             H11A1   -O11A    -H11A2      1_555  1_555  1_555     # 4721 Check
PLAT752_ALERT_4_C Angle   Calc       98.00, Rep     97.6(2) ......  Senseless s.u.
             H11B1   -O11B    -H11B2      1_555  1_555  1_555     # 4731 Check
PLAT752_ALERT_4_C Angle   Calc       91.00, Rep     90.8(2) ......  Senseless s.u.
             H12B1   -O12B    -H12B2      1_555  1_555  1_555     # 4747 Check
PLAT752_ALERT_4_C Angle   Calc       98.00, Rep     98.3(2) ......  Senseless s.u.
             H13A1   -O13A    -H13A2      1_555  1_555  1_555     # 4757 Check
PLAT752_ALERT_4_C Angle   Calc      134.00, Rep    134.0(3) ......  Senseless s.u.
             H13B1   -O13B    -H13B2      1_555  1_555  1_555     # 4767 Check
PLAT752_ALERT_4_C Angle   Calc      101.00, Rep    101.1(3) ......  Senseless s.u.
             H14A1   -O14A    -H14A2      1_555  1_555  1_555     # 4768 Check
PLAT752_ALERT_4_C Angle   Calc      105.00, Rep    104.5(3) ......  Senseless s.u.
             H14B1   -O14B    -H14B2      1_555  1_555  1_555     # 4769 Check
PLAT752_ALERT_4_C Angle   Calc      100.00, Rep     99.7(2) ......  Senseless s.u.
             H15A1   -O15A    -H15A2      1_555  1_555  1_555     # 4772 Check
PLAT752_ALERT_4_C Angle   Calc      118.00, Rep    118.5(3) ......  Senseless s.u.
             H15B1   -O15B    -H15B2      1_555  1_555  1_555     # 4775 Check
PLAT752_ALERT_4_C Angle   Calc       33.00, Rep   32.93(16) ......  Senseless s.u.
             O10B    -H10B1   -H10B2      1_555  1_555  1_555     # 4820 Check
PLAT752_ALERT_4_C Angle   Calc       37.00, Rep   36.56(18) ......  Senseless s.u.
             O10B    -H10B2   -H10B1      1_555  1_555  1_555     # 4830 Check
PLAT752_ALERT_4_C Angle   Calc       42.00, Rep   41.96(15) ......  Senseless s.u.
             O11A    -H11A1   -H11A2      1_555  1_555  1_555     # 4836 Check
PLAT752_ALERT_4_C Angle   Calc       38.00, Rep   37.62(15) ......  Senseless s.u.
             O11A    -H11A2   -H11A1      1_555  1_555  1_555     # 4846 Check
PLAT752_ALERT_4_C Angle   Calc       43.00, Rep   43.44(16) ......  Senseless s.u.
             O11B    -H11B1   -H11B2      1_555  1_555  1_555     # 4852 Check
PLAT752_ALERT_4_C Angle   Calc       39.00, Rep   38.97(16) ......  Senseless s.u.
             O11B    -H11B2   -H11B1      1_555  1_555  1_555     # 4862 Check
PLAT752_ALERT_4_C Angle   Calc       39.00, Rep   38.75(16) ......  Senseless s.u.
             O13A    -H13A1   -H13A2      1_555  1_555  1_555     # 4887 Check
PLAT752_ALERT_4_C Angle   Calc       43.00, Rep   42.93(16) ......  Senseless s.u.
             O13A    -H13A2   -H13A1      1_555  1_555  1_555     # 4908 Check
PLAT752_ALERT_4_C Angle   Calc       37.00, Rep   37.40(19) ......  Senseless s.u.
             O14A    -H14A1   -H14A2      1_555  1_555  1_555     # 4927 Check
PLAT752_ALERT_4_C Angle   Calc       42.00, Rep   41.50(18) ......  Senseless s.u.
             O14A    -H14A2   -H14A1      1_555  1_555  1_555     # 4928 Check
PLAT752_ALERT_4_C Angle   Calc       40.00, Rep   40.27(16) ......  Senseless s.u.
             O14B    -H14B1   -H14B2      1_555  1_555  1_555     # 4929 Check
PLAT752_ALERT_4_C Angle   Calc       35.00, Rep   35.24(15) ......  Senseless s.u.
             O14B    -H14B2   -H14B1      1_555  1_555  1_555     # 4930 Check
PLAT755_ALERT_4_C D-H     Calc     1.04000, Rep    1.043(3) ......  Senseless s.u.
             O9A      -H9A1           1_555   1_555 ........     #    7 Check
PLAT755_ALERT_4_C D-H     Calc     1.04000, Rep    1.043(3) ......  Senseless s.u.
             O9A      -H9A1           1_555   1_555 ........     #    8 Check
PLAT755_ALERT_4_C D-H     Calc     0.91000, Rep    0.912(2) ......  Senseless s.u.
             O9A      -H9A2           1_555   1_555 ........     #    9 Check
PLAT755_ALERT_4_C D-H     Calc     0.85000, Rep    0.851(3) ......  Senseless s.u.
             O9B      -H9B1           1_555   1_555 ........     #   10 Check
PLAT755_ALERT_4_C D-H     Calc     1.06000, Rep    1.056(2) ......  Senseless s.u.
             O9B      -H9B2           1_555   1_555 ........     #   11 Check
PLAT755_ALERT_4_C D-H     Calc     0.78000, Rep    0.781(2) ......  Senseless s.u.
             O10A     -H10A1          1_555   1_555 ........     #   12 Check
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PLAT755_ALERT_4_C D-H     Calc     0.85000, Rep    0.847(2) ......  Senseless s.u.
             O10B     -H10B1          1_555   1_555 ........     #   13 Check
PLAT755_ALERT_4_C D-H     Calc     0.77000, Rep    0.773(2) ......  Senseless s.u.
             O10B     -H10B2          1_555   1_555 ........     #   14 Check
PLAT755_ALERT_4_C D-H     Calc     0.84000, Rep    0.837(3) ......  Senseless s.u.
             O11A     -H11A1          1_555   1_555 ........     #   15 Check
PLAT755_ALERT_4_C D-H     Calc     0.92000, Rep    0.917(2) ......  Senseless s.u.
             O11A     -H11A2          1_555   1_555 ........     #   16 Check
PLAT755_ALERT_4_C D-H     Calc     0.92000, Rep    0.917(2) ......  Senseless s.u.
             O11A     -H11A2          1_555   1_555 ........     #   17 Check
PLAT755_ALERT_4_C D-H     Calc     0.79000, Rep    0.787(3) ......  Senseless s.u.
             O11B     -H11B1          1_555   1_555 ........     #   18 Check
PLAT755_ALERT_4_C D-H     Calc     0.86000, Rep    0.861(2) ......  Senseless s.u.
             O11B     -H11B2          1_555   1_555 ........     #   19 Check
PLAT755_ALERT_4_C D-H     Calc     0.86000, Rep    0.861(2) ......  Senseless s.u.
             O11B     -H11B2          1_555   1_555 ........     #   20 Check
PLAT755_ALERT_4_C D-H     Calc     0.84000, Rep    0.844(2) ......  Senseless s.u.
             O12A     -H12A1          1_555   1_555 ........     #   21 Check
PLAT755_ALERT_4_C D-H     Calc     0.93000, Rep    0.927(2) ......  Senseless s.u.
             O12B     -H12B1          1_555   1_555 ........     #   22 Check
PLAT755_ALERT_4_C D-H     Calc     0.93000, Rep    0.927(2) ......  Senseless s.u.
             O12B     -H12B1          1_555   1_555 ........     #   23 Check
PLAT755_ALERT_4_C D-H     Calc     1.03000, Rep    1.028(2) ......  Senseless s.u.
             O12B     -H12B2          1_555   1_555 ........     #   24 Check
PLAT755_ALERT_4_C D-H     Calc     0.90000, Rep    0.902(2) ......  Senseless s.u.
             O13A     -H13A1          1_555   1_555 ........     #   25 Check
PLAT755_ALERT_4_C D-H     Calc     0.83000, Rep    0.829(3) ......  Senseless s.u.
             O13A     -H13A2          1_555   1_555 ........     #   26 Check
PLAT755_ALERT_4_C D-H     Calc     0.83000, Rep    0.829(3) ......  Senseless s.u.
             O13A     -H13A2          1_555   1_555 ........     #   27 Check
PLAT755_ALERT_4_C D-H     Calc     0.83000, Rep    0.829(3) ......  Senseless s.u.
             O13A     -H13A2          1_555   1_555 ........     #   28 Check
PLAT755_ALERT_4_C D-H     Calc     0.90000, Rep    0.902(3) ......  Senseless s.u.
             O13B     -H13B1          1_555   1_555 ........     #   29 Check
PLAT755_ALERT_4_C D-H     Calc     0.90000, Rep    0.902(3) ......  Senseless s.u.
             O13B     -H13B1          1_555   1_555 ........     #   30 Check
PLAT755_ALERT_4_C D-H     Calc     0.90000, Rep    0.902(3) ......  Senseless s.u.
             O13B     -H13B1          1_555   1_555 ........     #   31 Check
PLAT755_ALERT_4_C D-H     Calc     1.11000, Rep    1.114(3) ......  Senseless s.u.
             O13B     -H13B2          1_555   1_555 ........     #   32 Check
PLAT755_ALERT_4_C D-H     Calc     0.81000, Rep    0.808(2) ......  Senseless s.u.
             O14A     -H14A1          1_555   1_555 ........     #   33 Check
PLAT755_ALERT_4_C D-H     Calc     0.74000, Rep    0.741(3) ......  Senseless s.u.
             O14A     -H14A2          1_555   1_555 ........     #   34 Check
PLAT755_ALERT_4_C D-H     Calc     0.74000, Rep    0.741(3) ......  Senseless s.u.
             O14A     -H14A2          1_555   1_555 ........     #   35 Check
PLAT755_ALERT_4_C D-H     Calc     0.77000, Rep    0.772(2) ......  Senseless s.u.
             O14B     -H14B1          1_555   1_555 ........     #   36 Check
PLAT755_ALERT_4_C D-H     Calc     0.86000, Rep    0.865(2) ......  Senseless s.u.
             O14B     -H14B2          1_555   1_555 ........     #   37 Check
PLAT755_ALERT_4_C D-H     Calc     1.07000, Rep    1.069(2) ......  Senseless s.u.
             O15A     -H15A2          1_555   1_555 ........     #   38 Check
PLAT755_ALERT_4_C D-H     Calc     1.07000, Rep    1.069(2) ......  Senseless s.u.
             O15A     -H15A2          1_555   1_555 ........     #   39 Check
PLAT755_ALERT_4_C D-H     Calc     0.85000, Rep    0.846(2) ......  Senseless s.u.
             O15B     -H15B1          1_555   1_555 ........     #   40 Check
PLAT755_ALERT_4_C D-H     Calc     0.85000, Rep    0.851(3) ......  Senseless s.u.
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              O15B     -H15B2          1_555   1_555 .......     #   41 Check
PLAT756_ALERT_4_C H...A   Calc     2.49000, Rep    2.486(3) ......  Senseless s.u.
              HA1A     -O12B          1_555   4_555 .......     #    1 Check
PLAT756_ALERT_4_C H...A   Calc     2.43000, Rep    2.433(3) ......  Senseless s.u.
              HA1A     -O15B          1_555   3_764 .......     #    2 Check
PLAT756_ALERT_4_C H...A   Calc     2.49000, Rep    2.486(3) ......  Senseless s.u.
              HA1A     -O12B          1_555   4_555 .......     #    3 Check
PLAT756_ALERT_4_C H...A   Calc     2.43000, Rep    2.433(3) ......  Senseless s.u.
              HA1A     -O15B          1_555   3_764 .......     #    4 Check
PLAT756_ALERT_4_C H...A   Calc     1.92000, Rep    1.923(2) ......  Senseless s.u.
              HA1B     -O7A           1_555   4_564 .......     #    5 Check
PLAT756_ALERT_4_C H...A   Calc     1.92000, Rep    1.923(2) ......  Senseless s.u.
              HA1B     -O7A           1_555   4_564 .......     #    6 Check
PLAT756_ALERT_4_C H...A   Calc     2.45000, Rep  2.4488(15) ......  Senseless s.u.
              H9A1     -P2B           1_555   4_455 .......     #    7 Check
PLAT756_ALERT_4_C H...A   Calc     1.64000, Rep    1.640(3) ......  Senseless s.u.
              H9A1     -O5B           1_555   4_455 .......     #    8 Check
PLAT756_ALERT_4_C H...A   Calc     2.26000, Rep    2.257(2) ......  Senseless s.u.
              H9A2     -O1B           1_555   1_466 .......     #    9 Check
PLAT756_ALERT_4_C H...A   Calc     1.86000, Rep    1.856(3) ......  Senseless s.u.
              H9B1     -O5A           1_555   4_554 .......     #   10 Check
PLAT756_ALERT_4_C H...A   Calc     1.89000, Rep    1.886(2) ......  Senseless s.u.
              H9B2     -O6B           1_555   1_555 .......     #   11 Check
PLAT756_ALERT_4_C H...A   Calc     2.24000, Rep    2.235(2) ......  Senseless s.u.
              H10A1    -O14B          1_555   4_555 .......     #   12 Check
PLAT756_ALERT_4_C H...A   Calc     1.97000, Rep    1.968(3) ......  Senseless s.u.
              H10B1    -O12B          1_555   4_545 .......     #   13 Check
PLAT756_ALERT_4_C H...A   Calc     2.00000, Rep    1.999(3) ......  Senseless s.u.
              H10B2    -O14A          1_555   4_654 .......     #   14 Check
PLAT756_ALERT_4_C H...A   Calc     1.99000, Rep    1.993(3) ......  Senseless s.u.
              H11A1    -O1A           1_555   4_564 .......     #   15 Check
PLAT756_ALERT_4_C H...A   Calc     2.02000, Rep    2.018(2) ......  Senseless s.u.
              H11A2    -O2B           1_555   1_466 .......     #   16 Check
PLAT756_ALERT_4_C H...A   Calc     2.36000, Rep    2.358(3) ......  Senseless s.u.
              H11A2    -O4A           1_555   4_564 .......     #   17 Check
PLAT756_ALERT_4_C H...A   Calc     1.94000, Rep    1.940(3) ......  Senseless s.u.
              H11B1    -O1B           1_555   4_545 .......     #   18 Check
PLAT756_ALERT_4_C H...A   Calc     2.02000, Rep    2.020(2) ......  Senseless s.u.
              H11B2    -O2A           1_555   1_544 .......     #   19 Check
PLAT756_ALERT_4_C H...A   Calc     2.42000, Rep    2.417(3) ......  Senseless s.u.
              H11B2    -O4B           1_555   4_545 .......     #   20 Check
PLAT756_ALERT_4_C H...A   Calc     1.98000, Rep    1.983(3) ......  Senseless s.u.
              H12A1    -O10A          1_555   4_565 .......     #   21 Check
PLAT756_ALERT_4_C H...A   Calc     1.73000, Rep    1.735(2) ......  Senseless s.u.
              H12B2    -O14B          1_555   1_555 .......     #   24 Check
PLAT756_ALERT_4_C H...A   Calc     1.78000, Rep    1.785(3) ......  Senseless s.u.
              H13A1    -O15A          1_555   1_555 .......     #   25 Check
PLAT756_ALERT_4_C H...A   Calc     2.36000, Rep    2.364(2) ......  Senseless s.u.
              H13A2    -X2            1_555   2_755 .......     #   26 Check
PLAT756_ALERT_4_C H...A   Calc     2.16000, Rep    2.161(3) ......  Senseless s.u.
              H13A2    -O3A           1_555   1_555 .......     #   27 Check
PLAT756_ALERT_4_C H...A   Calc     2.37000, Rep    2.365(3) ......  Senseless s.u.
              H13A2    -O7B           1_555   2_755 .......     #   28 Check
PLAT756_ALERT_4_C H...A   Calc     2.50000, Rep    2.495(2) ......  Senseless s.u.
              H13B1    -X1            1_555   2_744 .......     #   29 Check
PLAT756_ALERT_4_C H...A   Calc     2.15000, Rep    2.152(3) ......  Senseless s.u.
              H13B1    -O3B           1_555   1_555 .......     #   30 Check
```

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PLAT756_ALERT_4_C H...A   Calc     2.23000, Rep    2.227(3) ......  Senseless s.u.
             H13B1    -O7A            1_555   2_744 ........     #   31 Check
PLAT756_ALERT_4_C H...A   Calc     1.61000, Rep    1.606(3) ......  Senseless s.u.
             H13B2    -O15B           1_555   1_555 ........     #   32 Check
PLAT756_ALERT_4_C H...A   Calc     1.98000, Rep    1.982(2) ......  Senseless s.u.
             H14A1    -O8B            1_555   4_455 ........     #   33 Check
PLAT756_ALERT_4_C H...A   Calc     2.42000, Rep    2.417(2) ......  Senseless s.u.
             H14A2    -O3B            1_555   4_456 ........     #   34 Check
PLAT756_ALERT_4_C H...A   Calc     2.37000, Rep    2.373(3) ......  Senseless s.u.
             H14A2    -O12A           1_555   1_555 ........     #   35 Check
PLAT756_ALERT_4_C H...A   Calc     2.08000, Rep    2.080(2) ......  Senseless s.u.
             H14B1    -O3A            1_555   4_553 ........     #   36 Check
PLAT756_ALERT_4_C H...A   Calc     1.93000, Rep    1.933(2) ......  Senseless s.u.
             H14B2    -O8A            1_555   4_554 ........     #   37 Check
PLAT756_ALERT_4_C H...A   Calc     1.77000, Rep    1.772(2) ......  Senseless s.u.
             H15A2    -O2B            1_555   2_755 ........     #   38 Check
PLAT756_ALERT_4_C H...A   Calc     2.38000, Rep    2.381(3) ......  Senseless s.u.
             H15A2    -O13A           1_555   3_667 ........     #   39 Check
PLAT756_ALERT_4_C H...A   Calc     2.09000, Rep    2.089(2) ......  Senseless s.u.
             H15B1    -O2A            1_555   2_744 ........     #   40 Check
PLAT756_ALERT_4_C H...A   Calc     2.33000, Rep    2.333(3) ......  Senseless s.u.
             H15B2    -O14A           1_555   2_644 ........     #   41 Check
PLAT758_ALERT_4_C D-H..A  Calc      161.00, Rep  161.22(15) ......  Senseless s.u.
             O9B     -H9B2    -O6B        1_555  1_555  1_555     #   11 Check
PLAT758_ALERT_4_C D-H..A  Calc      172.00, Rep  171.83(15) ......  Senseless s.u.
             O12B    -H12B2   -O14B       1_555  1_555  1_555     #   24 Check
PLAT758_ALERT_4_C D-H..A  Calc      166.00, Rep  165.66(18) ......  Senseless s.u.
             O13A    -H13A1   -O15A       1_555  1_555  1_555     #   25 Check
PLAT758_ALERT_4_C D-H..A  Calc      138.00, Rep  137.65(17) ......  Senseless s.u.
             O13A    -H13A2   -O3A        1_555  1_555  1_555     #   27 Check
PLAT758_ALERT_4_C D-H..A  Calc      147.00, Rep  146.72(15) ......  Senseless s.u.
             O13B    -H13B1   -O3B        1_555  1_555  1_555     #   30 Check
PLAT758_ALERT_4_C D-H..A  Calc      163.00, Rep  162.83(16) ......  Senseless s.u.
             O13B    -H13B2   -O15B       1_555  1_555  1_555     #   32 Check
PLAT758_ALERT_4_C D-H..A  Calc      116.00, Rep  115.93(19) ......  Senseless s.u.
             O14A    -H14A2   -O12A       1_555  1_555  1_555     #   35 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:H28 Al1.835 Fe0.683 K0.962 Mg0.2
           Atom count from the _atom_site data:  H28 Al1.8375 Fe0.687 K0.956 Mg0.
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: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  H28 O32.958 Mg0.255 Al1.835 P4 K0.
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H        112.00    112.00    0.00
          O        131.83    131.86   -0.02
          Mg         1.02      1.06   -0.04
          Al         7.34      7.35   -0.01
          P         16.00     16.00    0.00
```

```
          K          3.85      3.82    0.02
          Ti         1.93      1.90    0.03
          Mn         6.98      6.94    0.04
          Fe         2.73      2.75   -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 ..............         28 Report
             Ha1A  Ha1B  H9A1  H9A2  H9B1  H9B2  H10A1 H10B1 H10B2 H11A1 H11A2
             H11B1 H11B2 H12A1 H12B1 H12B2 H13A1 H13A2 H13B1 H13B2 H14A1 H14A2
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A1     as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1B1     as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A2     as         MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1B2     as         MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A1     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B1     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A2     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B2     as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A1     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B1     as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A2     as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B2     as         TI
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         88 %Fit
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        18% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    7)       100% Note
PLAT303_ALERT_2_G Full Occupancy Atom H9A2      with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H12B1     with # Connections       1.00 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         44 Note
             M1A1    M1B1    M1A2    M1B2    M2A1    M2B1    M2A2    M2B2
             M3A1    M3B1    M3A2    M3B2    Ow1     Ow2     X1      X2
             Ha1A    Ha1B    H9A1    H9A2    H9B1    H9B2    H10A1   H10B1
             H10B2   H11A1   H11A2   H11B1   H11B2   H12A1   H12B1   H12B2
             H13A1   H13A2   H13B1   H13B2   H14A1   H14A2   H14B1   H14B2
             H15A1   H15A2   H15B1   H15B2
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 !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
PLAT982_ALERT_1_G The Al-f'=    0.0659 Deviates from  IT-value =       0.0645 Check
PLAT982_ALERT_1_G The Fe-f'=    0.3486 Deviates from  IT-value =       0.3463 Check
PLAT982_ALERT_1_G The  K-f'=    0.2025 Deviates from  IT-value =       0.2009 Check
PLAT982_ALERT_1_G The Mg-f'=    0.0503 Deviates from  IT-value =       0.0486 Check
PLAT982_ALERT_1_G The Mn-f'=    0.3394 Deviates from  IT-value =       0.3368 Check
PLAT982_ALERT_1_G The  P-f'=    0.1041 Deviates from  IT-value =       0.1023 Check
PLAT982_ALERT_1_G The Ti-f'=    0.2808 Deviates from  IT-value =       0.2776 Check
PLAT983_ALERT_1_G The Al-f"=    0.0526 Deviates from  IT-Value =       0.0514 Check
PLAT983_ALERT_1_G The Fe-f"=    0.8535 Deviates from  IT-Value =       0.8444 Check
PLAT983_ALERT_1_G The  K-f"=    0.2536 Deviates from  IT-Value =       0.2494 Check
PLAT983_ALERT_1_G The Mg-f"=    0.0374 Deviates from  IT-Value =       0.0363 Check
PLAT983_ALERT_1_G The Mn-f"=    0.7370 Deviates from  IT-Value =       0.7283 Check
PLAT983_ALERT_1_G The  P-f"=    0.0961 Deviates from  IT-Value =       0.0942 Check
PLAT983_ALERT_1_G The Ti-f"=    0.4522 Deviates from  IT-Value =       0.4457 Check
```

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

  37 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
 142 ALERT type 4 Improvement, methodology, query or suggestion
   5 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_PLAT112_I
;
PROBLEM: ADDSYM Detects New (Pseudo) Symm. Elem         a        100 %Fit
RESPONSE: ...
;
_vrf_PLAT113_I
;
PROBLEM: ADDSYM Suggests Possible Pseudo/New  Space Group       Pbca Check
RESPONSE: ...
;
_vrf_PLAT355_I
;
PROBLEM: Long   O-H (X0.82,N0.98A)  O13B     - H13B2    .       1.11 Ang.
RESPONSE: ...
;
_vrf_PLAT416_I
;
PROBLEM: Short Intra D-H..H-D       Ha1A     ..H12B1    .       1.64 Ang.
RESPONSE: ...
;
_vrf_PLAT417_I
;
PROBLEM: Short Inter D-H..H-D       H12B2    ..H14B1    .       2.04 Ang.
RESPONSE: ...
;
_vrf_PLAT420_I
;
PROBLEM: D-H Bond Without Acceptor  O12B     --H12B1    .     Please Check
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
```

```
;
_vrf_PLAT051_I
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.67 %
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_PLAT314_I
;
PROBLEM: Small Angle for H2O: Metal-O9A      -H9A2      .      45.85 Degree
RESPONSE: ...
;
_vrf_PLAT751_I
;
PROBLEM: Bond    Calc     1.04000, Rep    1.043(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT752_I
;
PROBLEM: Angle   Calc       99.00, Rep     99.3(2) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT755_I
;
PROBLEM: D-H     Calc     1.04000, Rep    1.043(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT756_I
;
PROBLEM: H...A   Calc     2.49000, Rep    2.486(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT758_I
;
PROBLEM: D-H..A  Calc      161.00, Rep  161.22(15) ......  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 06/01/2024; check.def file version of 05/01/2024

Datablock I - ellipsoid plot