checkCIF/PLATON report

Bond distances and angles from GSAS-II had incorrect unit cell offsets prior to GSAS-II version 4876. The GSAS-II authors recommend updating. If a CIF file from the most recent GSAS-II version is still showing problems, you are encouraged to contact the software authors.

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: CaWO,N3_phase_0

```
Bond precision:    = 0.0000 A                 Wavelength=0.71073

Cell:              a=5.57079(11)     b=7.85971(17)      c=5.53262(10)
                   alpha=90          beta=90            gamma=90
Temperature:       298 K

                   Calculated                Reported
Volume             242.245(8)                242.245(5)
Space group        P n m a                   P n m a
Hall group         -P 2ac 2n                 -P 2ac 2n
Moiety formula     N3 O3 W2, 2(Ca)           ?
Sum formula        Ca2 N3 O3 W2              Ca N1.5 O1.5 W
Mr                 537.87                    268.94
Dx,g cm-3          7.374                     7.374
Z                  2                         4
Mu (mm-1)          49.484                    0.000
F000               466.0                     0.0
F000'              464.27
h,k,lmax
Nref
Tmin,Tmax
Tmin'


Correction method= Not given


Data completeness=                    Theta(max)=
```

```
R(reflections)=                                           wR2(reflections)=
S =                         Npar=
```

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 A**

```
PLAT702_ALERT_1_A Angle   Calc   117.15(5), Rep   86.22(11), Dev..    618.60 Sigma
             O1      -CA1     -O1        1_555  1_555  6_666     #    1 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc  126.38(10), Rep  125.43(7), Dev..      9.50 Sigma
             O1      -CA1     -O2        6_666  1_555  1_555     #    3 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc    72.58(5), Rep  125.43(7), Dev..   1057.00 Sigma
             O1      -CA1     -O2        6_666  1_555  3_555     #    5 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   115.38(6), Rep   63.28(6), Dev..    868.33 Sigma
             O1      -CA1     -O2        6_666  1_555  5_656     #    8 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc    83.76(2), Rep   66.00(8), Dev..    888.00 Sigma
             O1      -CA1     -O2        1_555  1_555  7_666     #   11 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc    49.97(1), Rep   63.28(6), Dev..   1331.00 Sigma
             O1      -CA1     -O2        6_666  1_555  7_666     #   12 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   144.14(7), Rep  170.48(9), Dev..    376.29 Sigma
             O2      -CA1     -O2        1_555  1_555  7_666     #   13 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   53.83(4), Rep   80.70(3), Dev..    671.83 Sigma
           O2      -CA1     -O2        3_555  1_555  7_666     #   14 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc  135.01(8), Rep  108.07(11), Dev..    336.75 Sigma
           O2      -CA1     -O2        5_656  1_555  7_666     #   15 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   84.90(4), Rep   90.18(6), Dev..    132.00 Sigma
           O1      -W1      -O2        1_555  1_555  8_656     #   26 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   95.10(4), Rep   89.82(6), Dev..    132.00 Sigma
           O1      -W1      -O2        5_655  1_555  8_656     #   27 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   57.06(3), Rep  101.06(11), Dev..   1466.67 Sigma
           CA1     -O1      -CA1       1_555  1_555  6_566     #   31 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc  149.73(5), Rep   90.45(5), Dev..   1185.60 Sigma
           CA1     -O1      -W1        6_566  1_555  1_555     #   33 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   45.02(3), Rep   90.45(5), Dev..   1514.33 Sigma
           CA1     -O1      -W1        6_566  1_555  3_555     #   35 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc   57.06(3), Rep  101.06(9), Dev..   1466.67 Sigma
           CA1     -N1      -CA1       1_555  1_555  6_566     #   43 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc  149.73(5), Rep   90.45(1), Dev..   1185.66 Sigma
           CA1     -N1      -W1        6_566  1_555  1_555     #   45 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT702_ALERT_1_A Angle   Calc    45.02(3), Rep    90.45(1), Dev..   1514.23 Sigma
                CA1     -N1     -W1        6_566 1_555 3_555    #   47 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT722_ALERT_1_A Angle   Calc   156.14(2), Rep       89.59 Dev...      66.55 Degree
                O2      -W1     -O2        1_554 1_555 8_656    #   28 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT722_ALERT_1_A Angle   Calc   112.79(3), Rep      180.00 Dev...      67.21 Degree
                O2      -W1     -O2        4_554 1_555 8_656    #   29 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT722_ALERT_1_A Angle   Calc    23.86(2), Rep       90.41 Dev...      66.55 Degree
                O2      -W1     -O2        5_656 1_555 8_656    #   30 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

🟡 **Alert level C**
```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ    Please Check
                Calc: Ca N1.50 O1.50 W
                Rep.: Ca N1.5 O1.5 W
```

⚪ **Alert level G**
```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.500 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         3 Units
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        75% Note
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data    Please Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found    Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found    Please Check
```

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

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

Datablock: CaWO,N3_phase_1

Bond precision: W- O = 0.0003 A   Wavelength=0.71073

Cell: a=5.2636(5)   b=5.2636(5)   c=11.3536(18)
                   alpha=90   beta=90   gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	314.56(8)	314.55(11)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	O8 W2, 2(Ca)	?
Sum formula	Ca2 O8 W2	Ca O4 W
Mr	575.84	287.93
Dx,g cm-3	6.080	6.080
Z	2	4
Mu (mm-1)	38.174	0.000
F000	504.0	0.0
F000'	502.30	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness=   Theta(max)=

R(reflections)=   wR2(reflections)=
S =   Npar=

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 A
PLAT722_ALERT_1_A Angle   Calc   44.55(1), Rep   114.01 Dev...   69.46 Degree
            O2   -W1   -O2   4_444 1_555 10_444   #   2 Check

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT722_ALERT_1_A Angle   Calc    63.87(1), Rep     107.25 Dev...      43.38 Degree
              O2      -W1      -O2      5_555  1_555 10_444      #    3 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

```
PLAT722_ALERT_1_A Angle   Calc   134.05(1), Rep     107.25 Dev...      26.80 Degree
              O2      -W1      -O2     10_444  1_555 15_545      #    6 Check
```

Author Response: Reported angles are correct. Calculated angles appear to be erroneous.

🟡 **Alert level C**
```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
              Calc: O8 W2, 2(Ca)
              Rep.: ?'
                                                    ,
PLAT741_ALERT_1_C Bond    Calc   2.4420(4), Rep     2.44193 ......    Missing s.u.
              CA0     -O2              1_555  1_555 ........      #    1 Check
PLAT741_ALERT_1_C Bond    Calc   2.4728(4), Rep     2.47282 ......    Missing s.u.
              CA0     -O2              1_555  2_445 ........      #    2 Check
PLAT741_ALERT_1_C Bond    Calc   2.4420(4), Rep     2.44193 ......    Missing s.u.
              CA0     -O2              1_555  6_545 ........      #    3 Check
PLAT741_ALERT_1_C Bond    Calc   2.4728(4), Rep     2.47282 ......    Missing s.u.
              CA0     -O2              1_555  7_455 ........      #    4 Check
PLAT741_ALERT_1_C Bond    Calc   2.4420(4), Rep     2.44193 ......    Missing s.u.
              CA0     -O2              1_555 11_545 ........      #    5 Check
PLAT741_ALERT_1_C Bond    Calc   2.4728(4), Rep     2.47282 ......    Missing s.u.
              CA0     -O2              1_555 12_555 ........      #    6 Check
PLAT741_ALERT_1_C Bond    Calc   2.4728(4), Rep     2.47282 ......    Missing s.u.
              CA0     -O2              1_555 13_545 ........      #    7 Check
PLAT741_ALERT_1_C Bond    Calc   2.4420(4), Rep     2.44193 ......    Missing s.u.
              CA0     -O2              1_555 16_445 ........      #    8 Check
PLAT741_ALERT_1_C Bond    Calc   1.8006(3), Rep     1.80058 ......    Missing s.u.
              W1      -O2              1_555  4_444 ........      #    9 Check
PLAT741_ALERT_1_C Bond    Calc   1.8006(3), Rep     1.80058 ......    Missing s.u.
              W1      -O2              1_555  5_555 ........      #   10 Check
PLAT741_ALERT_1_C Bond    Calc   1.8006(3), Rep     1.80058 ......    Missing s.u.
              W1      -O2              1_555 10_544 ........      #   11 Check
PLAT741_ALERT_1_C Bond    Calc   1.8006(3), Rep     1.80058 ......    Missing s.u.
              W1      -O2              1_555 15_545 ........      #   12 Check
PLAT741_ALERT_1_C Bond    Calc   2.4420(4), Rep     2.44193 ......    Missing s.u.
              O2      -CA0             1_555  1_555 ........      #   13 Check
PLAT741_ALERT_1_C Bond    Calc   2.4728(4), Rep     2.47282 ......    Missing s.u.
              O2      -CA0             1_555  4_544 ........      #   14 Check
PLAT741_ALERT_1_C Bond    Calc   1.8006(3), Rep     1.80058 ......    Missing s.u.
              O2      -W1              1_555  2_455 ........      #   15 Check
```

⚪ **Alert level G**
```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.500 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...      -3 Units
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........        1 Note
```

```
                  Ca0
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data      Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for W1            (V)       .     5.09 Info
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found      Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found      Please Check
```

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

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

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.
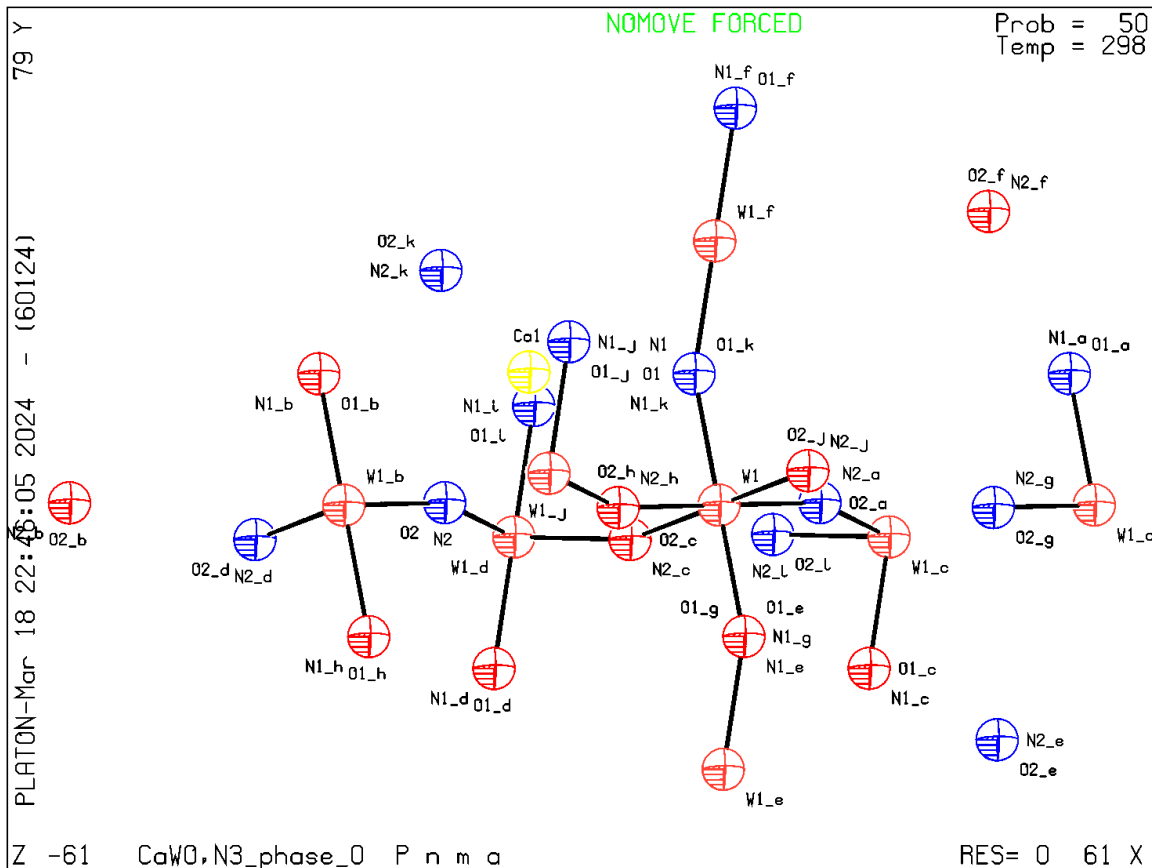
Publication of your CIF in IUCr journals

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 CaWO,N3_phase_0 ellipsoid plot. PLATON-Mar 18 22:46:05 2024 – (60124). NOMOVE FORCED. Prob = 50. Temp = 298. Z –61 CaWO,N3_phase_0 P n m a. RES= 0 61 X. 79 Y.

Datablock CaWO,N3_phase_1 - ellipsoid plot