checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ZDCW01-04

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: ZDCW01-04

```
Bond precision:   C-C = 0.0209 A           Wavelength=0.71075

Cell:           a=9.913(2)        b=9.930(2)         c=15.934(4)
                alpha=92.990(6)   beta=96.8585(10)   gamma=90.360(8)
Temperature:    125 K

                 Calculated                  Reported
Volume           1555.0(6)                   1555.0(6)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
Moiety formula   C31 H20 O10 P2 W2           C31 H20 O10 P2 W2
Sum formula      C31 H20 O10 P2 W2           C31 H20 O10 P2 W2
Mr               982.09                      982.14
Dx,g cm-3        2.098                       2.097
Z                2                           2
Mu (mm-1)        7.552                       7.560
F000             928.0                       928.0
F000'            925.60
h,k,lmax         11,11,19                    11,11,19
Nref             5694                        5547
Tmin,Tmax        0.223,0.298                 0.228,0.298
Tmin'            0.188

Correction method= # Reported T Limits: Tmin=0.228 Tmax=0.298
AbsCorr = MULTI-SCAN

Data completeness= 0.974            Theta(max)= 25.386

R(reflections)= 0.0705( 4913)                wR2(reflections)=
                                             0.2200( 5547)
S = 1.099                  Npar= 407
```

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

```
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       9.04 eA-3
```

Author Response: 4 crystals tried, best result presented -result fine for conclusions drawn- probably crystal quality issues.

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PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.02091 Ang.
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Author Response: 4 crystals tried, best result presented -result fine for conclusions drawn- probably crystal quality issues.

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PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          3 Check
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Author Response: Data left in for transparency purposes.

Alert level C

```
DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
            _refine_diff_density_min given =     -5.710
            Test value =     -5.550
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
            The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -5.71 eA-3
PLAT234_ALERT_4_C Large Hirshfeld Difference W2       --C30      .       0.16 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.140 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         88 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      13.69 Check
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Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          8 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      34.56 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         41 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
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PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        78% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         28 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law         [ 1-1 0] Est.d BASF       0.35 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        1.0 Low
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

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

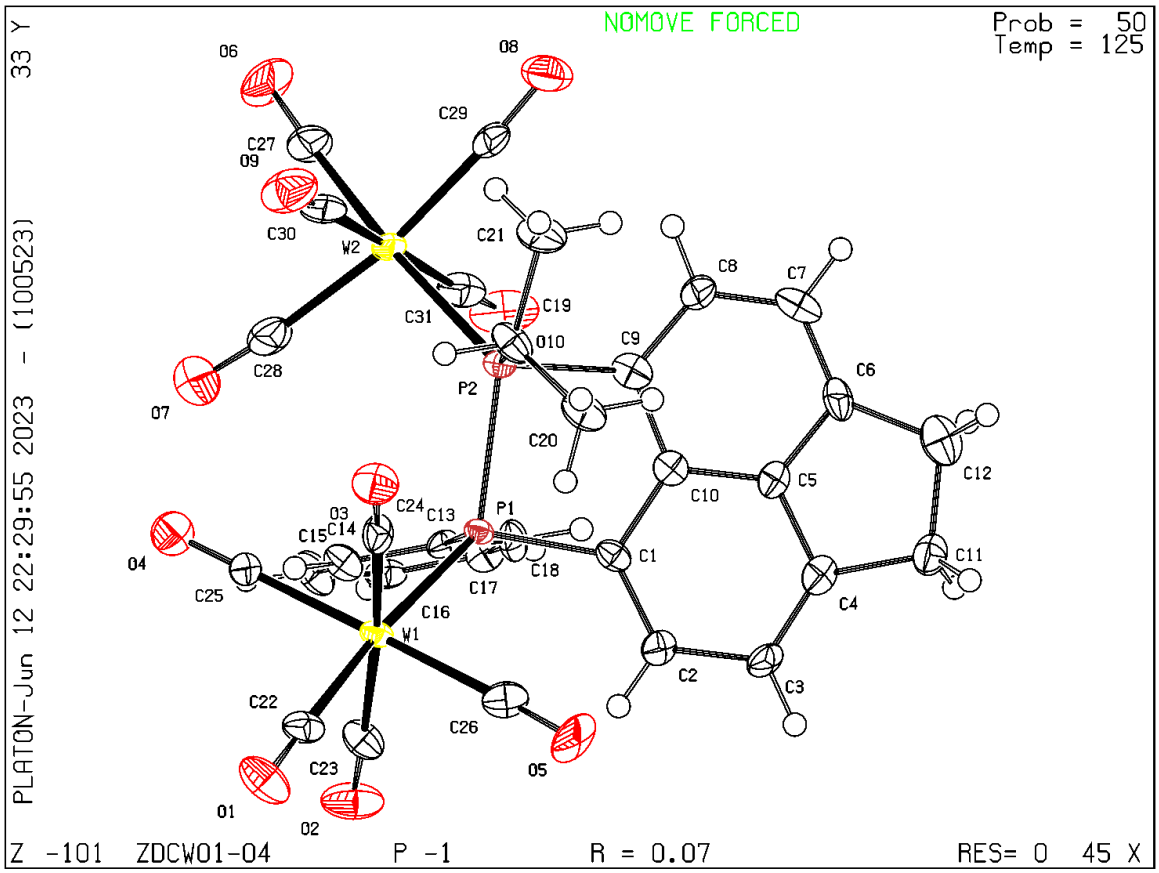
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 10/05/2023; check.def file version of 10/05/2023

Datablock ZDCW01-04 - ellipsoid plot