checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wcrnew

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: wcrnew

```
Bond precision:    C-C = 0.0607 A            Wavelength=0.71073

Cell:            a=23.323(5)       b=14.555(3)       c=17.009(7)
                 alpha=90          beta=90           gamma=90
Temperature:     296 K

                 Calculated                 Reported
Volume           5774(3)                    5774(3)
Space group      P c a 21                   P c a 21
Hall group       P 2c -2ac                  P 2c -2ac
Moiety formula   C24 H30 B4 Cr O4 W2        ?
Sum formula      C24 H30 B4 Cr O4 W2        C24 H37 B4 Cr O4 W2
Mr               845.40                     852.47
Dx,g cm-3        1.945                      1.961
Z                8                          8
Mu (mm-1)        8.345                      8.346
F000             3184.0                     3240.0
F000'            3175.05
h,k,lmax         27,16,19                   27,16,19
Nref             9617[ 4994]                8977
Tmin,Tmax        0.382,0.513                0.450,0.600
Tmin'            0.253

Correction method= # Reported T Limits: Tmin=0.450 Tmax=0.600
AbsCorr = MULTI-SCAN

Data completeness= 1.80/0.93      Theta(max)= 24.509

R(reflections)= 0.0879( 3645)      wR2(reflections)= 0.2215( 8977)

S = 0.997                   Npar= 650
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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**

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
          Rint given   0.274

> **Author Response: The crystal was poorly diffracting. This could have caused poor absorption profile. Also a small centrosymmetric twin componet (BASF 0.1)is present which makes the Rint further bad. Even after recrystallisation and fresh data collection the quality data did not much improve.**

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ....   0.274 Report

> **Author Response: The crystal was poorly diffracting. This could have caused poor absorption profile. Also a small centrosymmetric twin componet (BASF 0.1)is present which makes the Rint further bad. Even after recrystallisation and fresh data collection the quality data did not much improve.**

🟠 **Alert level B**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.06075 Ang.
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on   W2   1.52 eA-3

🟡 **Alert level C**

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =   0.5837
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..   41% Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   7.07 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ....   7.59 Note
PLAT147_ALERT_1_C s.u. on Symmetry Constrained Cell Angle(s) .....   Please Check
PLAT213_ALERT_2_C Atom C38   has ADP max/min Ratio .....   3.3 oblate
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C41 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Cr1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C43 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   W3 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   W4 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Cr2 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C22 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C45 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   W3   0.084 Check
PLAT723_ALERT_1_C Torsion Calc   -37.00, Rep   -34(34) Dev...   3.00 Sigma
         O1 -C41 -CR1 -C43   1.555   1.555   1.555   1.555 # 188 Check
PLAT723_ALERT_1_C Torsion Calc   56.00, Rep   59(34) Dev...   3.00 Sigma
         O1 -C41 -CR1 -C42   1.555   1.555   1.555   1.555 # 189 Check
PLAT723_ALERT_1_C Torsion Calc   -3.00, Rep   0(43) Dev...   3.00 Sigma
         O1 -C41 -CR1 -C44   1.555   1.555   1.555   1.555 # 190 Check
PLAT723_ALERT_1_C Torsion Calc   158.00, Rep   160(33) Dev...   2.00 Sigma
         O1 -C41 -CR1 -B1   1.555   1.555   1.555   1.555 # 191 Check
PLAT723_ALERT_1_C Torsion Calc   -154.00, Rep   -151(34) Dev...   3.00 Sigma

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                 O1  -C41 -CR1 -W1      1.555   1.555   1.555   1.555  #  192 Check
PLAT723_ALERT_1_C Torsion Calc        161.00, Rep       163(35) Dev...      2.00 Sigma
                 O1  -C41 -CR1 -W2      1.555   1.555   1.555   1.555  #  193 Check
PLAT733_ALERT_1_C Torsion Calc          -1(6), Rep       0.1(10) ......      6.00 s.u.-R
                 C8  -C3  -C4  -C9      1.555   1.555   1.555   1.555  #   20 Check
PLAT733_ALERT_1_C Torsion Calc        113(5), Rep     113.1(11) ......      4.55 s.u.-R
                 W2  -C11 -C12 -C17     1.555   1.555   1.555   1.555  #   44 Check
PLAT733_ALERT_1_C Torsion Calc       -179(4), Rep     -179.9(7) ......      5.71 s.u.-R
                 C22 -C23 -C24 -C29     1.555   1.555   1.555   1.555  #   94 Check
PLAT733_ALERT_1_C Torsion Calc          -1(4), Rep       0.0(7) ......      5.71 s.u.-R
                 C22 -C21 -C25 -C24     1.555   1.555   1.555   1.555  #  106 Check
PLAT733_ALERT_1_C Torsion Calc           1(4), Rep       0.1(8) ......      5.00 s.u.-R
                 C33 -C34 -C35 -C31     1.555   1.555   1.555   1.555  #  136 Check
PLAT733_ALERT_1_C Torsion Calc          -1(4), Rep       0.0(7) ......      5.71 s.u.-R
                 C32 -C31 -C35 -C34     1.555   1.555   1.555   1.555  #  144 Check
PLAT733_ALERT_1_C Torsion Calc           1(6), Rep      -0.2(10) ......      6.00 s.u.-R
                 C36 -C31 -C35 -C40     1.555   1.555   1.555   1.555  #  148 Check
PLAT753_ALERT_4_C Torsion Calc        -37.00, Rep       -34(34) ......    Senseless s.u.
                 O1  -C41 -CR1 -C43     1.555   1.555   1.555   1.555  #  188 Check
PLAT753_ALERT_4_C Torsion Calc         56.00, Rep        59(34) ......    Senseless s.u.
                 O1  -C41 -CR1 -C42     1.555   1.555   1.555   1.555  #  189 Check
PLAT753_ALERT_4_C Torsion Calc         -3.00, Rep         0(43) ......    Senseless s.u.
                 O1  -C41 -CR1 -C44     1.555   1.555   1.555   1.555  #  190 Check
PLAT753_ALERT_4_C Torsion Calc        158.00, Rep       160(33) ......    Senseless s.u.
                 O1  -C41 -CR1 -B1      1.555   1.555   1.555   1.555  #  191 Check
PLAT753_ALERT_4_C Torsion Calc       -154.00, Rep      -151(34) ......    Senseless s.u.
                 O1  -C41 -CR1 -W1      1.555   1.555   1.555   1.555  #  192 Check
PLAT753_ALERT_4_C Torsion Calc        161.00, Rep       163(35) ......    Senseless s.u.
                 O1  -C41 -CR1 -W2      1.555   1.555   1.555   1.555  #  193 Check
PLAT753_ALERT_4_C Torsion Calc        -48.00, Rep       -49(26) ......    Senseless s.u.
                 O5  -C45 -CR2 -C48     1.555   1.555   1.555   1.555  #  202 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.584         61 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         87 %
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.27A    From W4         1.77 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.24A    From W3         1.65 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       W1   1.46 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.92A    From O8        -0.66 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H29B        -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H36A        -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H40B        -0.41 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.     0 Info
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⬤ **Alert level G**

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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:C24 H37 B4 Cr1 O4 W2
            Atom count from the _atom_site data:  C24 H30 B4 Cr1 O4 W2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C24 H37 B4 Cr O4 W2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        192.00    192.00    0.00
          H        296.00    240.00   56.00
          B         32.00     32.00    0.00
          Cr         8.00      8.00    0.00
          O         32.00     32.00    0.00
          W         16.00     16.00    0.00
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        58 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        64 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         5 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        10 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         5 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C45 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C48 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C40 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C6        -H6B           1.555   1.555 ........     #   17 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C8        -H8C           1.555   1.555 ........     #   24 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C9        -H9A           1.555   1.555 ........     #   25 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C10       -H10B          1.555   1.555 ........     #   29 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C16       -H16A          1.555   1.555 ........     #   46 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C17       -H17C          1.555   1.555 ........     #   51 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C20       -H20C          1.555   1.555 ........     #   60 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C28       -H28B          1.555   1.555 ........     #   83 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C29       -H29A          1.555   1.555 ........     #   85 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C30       -H30A          1.555   1.555 ........     #   88 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C36       -H36B          1.555   1.555 ........     #  107 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C37       -H37B          1.555   1.555 ........     #  110 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C39       -H39A          1.555   1.555 ........     #  115 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
           C40       -H40C          1.555   1.555 ........     #  120 Check
PLAT722_ALERT_1_G Angle  Calc     108.00, Rep     109.50 Dev...      1.50 Degree
           H9A       -C9       -H9B      1.555  1.555  1.555  #   51 Check
PLAT722_ALERT_1_G Angle  Calc     111.00, Rep     109.50 Dev...      1.50 Degree
           C4        -C9       -H9C      1.555  1.555  1.555  #   52 Check
PLAT722_ALERT_1_G Angle  Calc     108.00, Rep     109.50 Dev...      1.50 Degree
           H20B      -C20      -H20C     1.555  1.555  1.555  #  120 Check
PLAT722_ALERT_1_G Angle  Calc     108.00, Rep     109.50 Dev...      1.50 Degree
           H30A      -C30      -H30B     1.555  1.555  1.555  #  177 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.20 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      666 Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  48 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

  37 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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25 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
17 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
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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 06/01/2019; check.def file version of 19/12/2018

NOMOVE FORCED

Prob = 50
Temp = 296

16 Y

PLATON-Jan 26 08:42:27 2019 - (70316)

Z -91   wcrnew   P c a 21   R = 0.09   RES=   0 -128 X