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: SGGF3

Bond precision: C-C = 0.0113 A   Wavelength=0.71073

Cell: a=16.3096(16)   b=18.8186(18)   c=19.9272(18)
               alpha=85.532(3)   beta=71.947(3)   gamma=89.111(3)
Temperature: 150 K

	Calculated	Reported
Volume	5797.1(10)	5797.1(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H30 B4 Mo O4 W2	C24 H30 B4 Mo O4 W2
Sum formula	C24 H30 B4 Mo O4 W2	C24 H30 B4 Mo O4 W2
Mr	889.34	889.36
Dx,g cm-3	2.038	2.038
Z	8	8
Mu (mm-1)	8.370	8.370
F000	3328.0	3328.0
F000'	3302.65	
h,k,lmax	21,24,25	21,24,25
Nref	26583	26525
Tmin,Tmax	0.168,0.433	0.246,0.433
Tmin'	0.127	

Correction method= # Reported T Limits: Tmin=0.246 Tmax=0.433
AbsCorr = MULTI-SCAN

Data completeness= 0.998   Theta(max)= 27.484

R(reflections)= 0.0349(22650)   wR2(reflections)= 0.0880(26525)

S = 1.065   Npar= 1295

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 C

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PLAT213_ALERT_2_C Atom O22              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C16              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C17              has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C18              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C22              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C38              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom O82              has ADP max/min Ratio .....        3.8 prolat
PLAT213_ALERT_2_C Atom C70              has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom C99              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C100             has ADP max/min Ratio .....        3.2 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 3  C   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 4  C   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Mo1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01131 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #        1 Note
              C24 H30 B4 Mo O4 W2
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Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      63.69 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.003 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1       --C23       .     5.7 s.u.
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for        C24 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for        C54 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for        C84 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for       C111 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C47 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O82      ..C43            2.94 Ang.
                                        x,y,z =      1_555 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.15 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        4 Note
              C24 H30 B4 Mo O4 W2
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  22 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 = 150

-39 Y

- (70316)

PLATON-Jan 23 15:05:48 2019

Z -100   SGGF3   P -1   R = 0.03   RES=   0 -141 X