checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:  C-C = 0.0109 A          Wavelength=1.54184

Cell:           a=10.3465(2)    b=19.1010(3)        c=15.1007(3)
                alpha=90        beta=105.009(2)     gamma=90
Temperature:    293 K

                Calculated                Reported
Volume          2882.52(10)               2882.52(10)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C31 H35 Cl2 O Os P        C31 H35 Cl2 O1 Os1 P1
Sum formula     C31 H35 Cl2 O Os P        C31 H35 Cl2 O Os P
Mr              715.69                    715.66
Dx,g cm-3       1.649                     1.649
Z               4                         4
Mu (mm-1)       10.751                    10.751
F000            1416.0                    1416.0
F000'           1402.71
h,k,lmax        12,23,18                  12,22,18
Nref            5436                      5321
Tmin,Tmax       0.159,0.179               0.761,1.000
Tmin'           0.061

Correction method= # Reported T Limits: Tmin=0.761 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.979          Theta(max)= 69.621

R(reflections)= 0.0407( 4587)     wR2(reflections)= 0.1033( 5321)

S = 1.065                 Npar= 319
```

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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .... 3 Report
C8A C9A C10A

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 4.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Os1 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01086 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.570 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.85A From Os1 -1.84 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77A From Os1 -1.58 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8A2 -0.35 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.25 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C1 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H15 ..H9B2 . 1.96 Ang.
-1+x,y,z = 1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C15 ..C9B 3.10 Ang.
-1+x,y,z = 1_455 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 8 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 4 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 89 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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 16/12/2019; check.def file version of 13/12/2019

Datablock shelx - ellipsoid plot