checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:  C-C = 0.0096 A          Wavelength=0.71073

Cell:            a=18.770(6)     b=13.876(4)          c=19.169(6)
                 alpha=90        beta=107.587(6)      gamma=90
Temperature:     296 K
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	Calculated	Reported
Volume	4759(3)	4759(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C48 H38 Cu N2 O P2, F6 P, C H2 Cl2	?
Sum formula	C49 H40 Cl2 Cu F6 N2 O P3	C49 H40 Cl2 Cu F6 N2 O P3
Mr	1014.19	1014.18
Dx,g cm-3	1.416	1.415
Z	4	4
Mu (mm-1)	0.734	0.734
F000	2072.0	2072.0
F000’	2076.57	
h,k,lmax	22,16,22	22,16,22
Nref	8412	8403
Tmin,Tmax	0.753,0.802	0.851,0.886
Tmin’	0.738	

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Correction method= # Reported T Limits: Tmin=0.851 Tmax=0.886
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.028

R(reflections)= 0.0654( 5451)     wR2(reflections)= 0.2000( 8403)

S = 1.030                  Npar= 596
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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 C

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1       --C12      .        7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27      --C48      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29      --C41      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P3       --F4       .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P3       --F5       .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P3       --F6       .       0.23 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C39 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C44 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C45 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C49 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        P3      0.223 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.217 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0096 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.802 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          9 Report
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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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.15 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --N1       .        5.7 s.u.
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6A        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        14% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             103.9 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        31% Note
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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
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  11 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 03/05/2019; check.def file version of 29/04/2019

Datablock 1 - ellipsoid plot