checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MEM011_130K

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: MEM011_130K

Bond precision: C-C = 0.0065 A   Wavelength=1.34143

Cell: a=10.4786(3)   b=18.9864(4)   c=22.1096(5)
               alpha=90   beta=100.077(2)   gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	4330.87(18)	4330.87(18)
Space group	P 21/c	P 21/c
Hall group	: -P 2ybc	-P 2ybc
Moiety formula	C47 H37 Cl Cu N2 O P2, F6 P	C47 H37 Cl1 Cu1 F6 N2 O1 P3
Sum formula	C47 H37 Cl Cu F6 N2 O P3	C47 H37 Cl1 Cu1 F6 N2 O1 P3
Mr	951.70	951.73
Dx,g cm-3	1.460	1.460
Z	4	4
Mu (mm-1)	4.150	4.150
F000	1944.0	1944.0
F000'	1941.36	
h,k,lmax	13,23,27	13,23,27
Nref	8920	8755
Tmin,Tmax	0.638,0.748	0.710,0.750
Tmin'	0.579	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.750
AbsCorr = NUMERICAL

Data completeness= 0.982   Theta(max)= 57.183

R(reflections)= 0.1124(7234)   wR2(reflections)= wR= 0.0443(7217)

S = 1.031   Npar= 539

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.

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Alert level B
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ....   6 Report
PLAT220_ALERT_2_B Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   10.0 Ratio

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Alert level C
PLAT082_ALERT_2_C High R1 Value ....   0.11 Report
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C60   .   6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C63   .   6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C62   .   6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C58   .   6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C61   .   6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C59   .   6 Check
PLAT222_ALERT_3_C Non-Solv. Resd 1 H   Uiso(max)/Uiso(min) Range   10.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C49 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C51 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   P3   0.134 Check
PLAT330_ALERT_2_C Large Aver Phenyl C-C Dist C52   -C64   .   1.41 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00648 Ang.
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   58 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   10 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .   18.98 Check

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Alert level G
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
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 ...   79 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C27   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C33   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C34   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43   Constrained at   0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C44        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C54        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C55        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C56        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C57        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C58        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C59        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C60        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C61        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C62        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C63        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C64        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C100       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C102       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1001      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1002      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1003      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1021      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1022      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1023      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H181       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H191       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H201       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H211       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H221       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H241       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H251       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H261       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H271       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H281       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H301       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H311       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H321       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H331       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H351       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H411       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H421       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H431       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H441       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H461       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H521       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H541       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H551       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H561       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H571       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H581       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H591       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H611       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H621       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H631       Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       37% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C102 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2       ..C42           2.94 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F4       ..C43           2.95 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       6 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found    Please Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      668 Note
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PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        1 Note
PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L=     0.600     1821 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      547 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked       ! Info
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
PLAT984_ALERT_1_G The Cu-f'=      -2.799 Deviates from the B&C-Value    -2.797   Ch
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
 16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 95 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
 15 ALERT type 3 Indicator that the structure quality may be low
 80 ALERT type 4 Improvement, methodology, query or suggestion
  4 ALERT type 5 Informative message, check
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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT082_MEM011_130K
;
PROBLEM: High R1 Value ................................     0.11 Report
RESPONSE: ...
;
_vrf_PLAT218_MEM011_130K
;
PROBLEM: Constrained U(ij) Components(s) for C60      .        6 Check
RESPONSE: ...
;
_vrf_PLAT222_MEM011_130K
;
PROBLEM: Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range     10.0 Ratio
RESPONSE: ...
;
_vrf_PLAT241_MEM011_130K
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of      C49 Check
RESPONSE: ...
;
_vrf_PLAT242_MEM011_130K
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of      C51 Check
RESPONSE: ...
;
_vrf_PLAT260_MEM011_130K
;
PROBLEM: Large Average Ueq of Residue Including       P3    0.134 Check
RESPONSE: ...
;
_vrf_PLAT330_MEM011_130K
;
PROBLEM: Large Aver Phenyl C-C Dist C52      -C64      .     1.41 Ang.
RESPONSE: ...
;
_vrf_PLAT341_MEM011_130K
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;
PROBLEM: Low Bond Precision on  C-C Bonds ..............     0.00648 Ang.
RESPONSE: ...
;
_vrf_PLAT913_MEM011_130K
;
PROBLEM: Missing # of Very Strong Reflections in FCF ....        58 Note
RESPONSE: ...
;
_vrf_PLAT918_MEM011_130K
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .        10 Check
RESPONSE: ...
;
_vrf_PLAT939_MEM011_130K
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .     18.98 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 19/10/2018; check.def file version of 15/10/2018

NOMOVE FORCED

Prob = 50
Temp = 130

38 Y

PLATON-Oct 26 09:57:43 2018 - (70316)

Z -26   MEM011_130P 21/c   R = 0.11   RES= 0   5 X