# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MEM012_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: MEM012_130K

Bond precision:   C-C = 0.0070 A           Wavelength=1.34143

Cell:        a=11.4363(6)       b=14.0871(6)       c=14.8030(7)
             alpha=89.133(4)   beta=68.457(4)   gamma=88.730(4)
Temperature:   130 K

|  | Calculated | Reported |
|---|---|---|
| Volume | 2217.62(19) | 2217.62(19) |
| Space group | P -1 | P -1 |
| Hall group | : -P 1 | -P 1 |
| Moiety formula | C50 H41 Cl Cu N2 O P2, F6 P | C50 H41 Cl1 Cu1 F6 N2 O1 P3 |
| Sum formula | C50 H41 Cl Cu F6 N2 O P3 | C50 H41 Cl1 Cu1 F6 N2 O1 P3 |
| Mr | 991.76 | 991.80 |
| Dx,g cm-3 | 1.485 | 1.485 |
| Z | 2 | 2 |
| Mu (mm-1) | 4.068 | 4.068 |
| F000 | 1016.0 | 1016.0 |
| F000' | 1014.75 | |
| h,k,lmax | 14,17,18 | 14,17,18 |
| Nref | 9159 | 8675 |
| Tmin,Tmax | | 0.880,0.890 |
| Tmin' | | |

Correction method= # Reported T Limits: Tmin=0.880 Tmax=0.890
AbsCorr = SPHERE

Data completeness= 0.947          Theta(max)= 57.215

R(reflections)= 0.1112( 7747)      wR2(reflections)= wR= 0.0483( 7713)

S = 0.994                  Npar= 573

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 C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
                   a literature citation. This should be contained in the
                   _exptl_absorpt_process_details field.
                   Absorption correction given as sphere
PLAT082_ALERT_2_C High R1 Value ...................................     0.11 Report
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       P3     0.116 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00698 Ang.
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....      16 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .       4 Check
PLAT920_ALERT_1_C Theta(Max)  in CIF and FCF Differ by ...........    0.42 Degree
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .   27.80 Check
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### ⚪ Alert level G

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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
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.004 Degree
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 C100        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C101        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 H1011       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1012       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1013       Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       4% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        2 Note
                  F6 P
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found  Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        2 Note
PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L=    0.600     1415 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      496 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
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  25 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
  14 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

## 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_ABSTY02_MEM012_130K
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT082_MEM012_130K
;
PROBLEM: High R1 Value ................................    0.11 Report
RESPONSE: ...
;
_vrf_PLAT250_MEM012_130K
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....     2.1 Note
RESPONSE: ...
;
_vrf_PLAT260_MEM012_130K
;
PROBLEM: Large Average Ueq of Residue Including       P3     0.116 Check
RESPONSE: ...
;
_vrf_PLAT341_MEM012_130K
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............   0.00698 Ang.
RESPONSE: ...
;
_vrf_PLAT913_MEM012_130K
;
PROBLEM: Missing # of Very Strong Reflections in FCF ....      16 Note
RESPONSE: ...
;
_vrf_PLAT918_MEM012_130K
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .       4 Check
RESPONSE: ...
;
_vrf_PLAT920_MEM012_130K
;
PROBLEM: Theta(Max)  in CIF and FCF Differ by ...........    0.42 Degree
RESPONSE: ...
;
_vrf_PLAT939_MEM012_130K
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .   27.80 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.

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

NOMOVE FORCED

Prob = 50
Temp = 130

11 Y

PLATON-Oct 25 17:53:18 2018 - (70316)

Z -134   MEM012_130P -1          R = 0.11              RES=   0   -91 X