checkCIF/PLATON report

Structure factors have been supplied for datablock(s) isn166_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: isn166_130k

Bond precision: C-C = 0.0098 A   Wavelength=1.34143

Cell: a=33.3182(16)   b=14.1050(6)   c=11.8205(5)
                 alpha=90   beta=102.059(4)   gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	5432.5(4)	5432.5(4)
Space group	C 2/m	C 1 2/m 1
Hall group	-C 2y	-C 2y
Moiety formula	C51 H38 Br2 Cu N2 O P2, F6 P [+ solvent]	0.5(C102 H76 Br4 Cu2 N4 O2 P4), F6 P, 1.1[CH2CL2]
Sum formula	C51 H38 Br2 Cu F6 N2 O P3 [+ solvent]	C52.10 H40.20 Br2 Cl2.20 Cu F6 N2 O P3
Mr	1125.09	1218.52
Dx,g cm-3	1.376	1.490
Z	4	4
Mu (mm-1)	4.173	4.895
F000	2256.0	2441.0
F000'	2244.77	
h,k,lmax	41,17,14	41,17,14
Nref	5751	5607
Tmin,Tmax	0.441,0.822	0.005,0.909
Tmin'	0.256	

Correction method= # Reported T Limits: Tmin=0.005 Tmax=0.909
AbsCorr = MULTI-SCAN

Data completeness= 0.975   Theta(max)= 56.714

R(reflections)= 0.0728(4802)   wR2(reflections)= 0.1973(5607)

S = 1.034   Npar= 417

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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PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including         P3     0.106 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........       C10 Check
PLAT332_ALERT_2_C Large Phenyl C-C Range     C13         -C37      .    0.17 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00985 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        43 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        6 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H10             -0.34 eA-3
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⚪ Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C52.1 H40.2 Br2 Cl2.2 Cu1 F6 N2
            Atom count from the _atom_site data:  C51 H38 Br2 Cu1 F6 N2 O1 P3
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
            not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C52.10 H40.20 Br2 Cl2.20 Cu F6 N2
           TEST: Compare cell contents of formula and atom_site data

           atom     Z*formula   cif sites  diff
           C         208.40     204.00     4.40
           H         160.80     152.00     8.80
           Br          8.00       8.00     0.00
           Cl          8.80       0.00     8.80
           Cu          4.00       4.00     0.00
           F          24.00      24.00     0.00
           N           8.00       8.00     0.00
           O           4.00       4.00     0.00
           P          12.00      12.00     0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         17 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         19 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ  Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   14.75 %
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   41.98 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records        2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for     C13        --C32      .    5.1 s.u.
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12        Constrained at      0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C14         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16         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 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 C29         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 C35         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C36         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C37         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H36         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37         Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )       47% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H9       ..H10      .    2.07 Ang.
                                             x,y,z =     1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure      441 A**3
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C8        --C9          1.96 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C9        --C8          1.96 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C33       --C33         2.02 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      136 Check
          C8  -C8  -C9     6.565   1.555   6.565              43.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      140 Check
          C9  -C8  -C9     1.555   1.555   6.565              39.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      151 Check
          C9  -C9  -C8     6.565   1.555   6.565              43.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      165 Check
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                  C33  -C33  -H33      6.565  1.555  1.555              15.10 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      156 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed        ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       99 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 Info
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value    0.0137 Check
PLAT984_ALERT_1_G The Br-f'=   -0.9501 Deviates from the B&C-Value   -0.9338 Check
PLAT984_ALERT_1_G The Cu-f'=   -2.9183 Deviates from the B&C-Value   -2.7974 Check
PLAT984_ALERT_1_G The  F-f'=    0.0600 Deviates from the B&C-Value    0.0583 Check
PLAT984_ALERT_1_G The  N-f'=    0.0253 Deviates from the B&C-Value    0.0241 Check
PLAT984_ALERT_1_G The  O-f'=    0.0412 Deviates from the B&C-Value    0.0389 Check
PLAT984_ALERT_1_G The  P-f'=    0.2596 Deviates from the B&C-Value    0.2543 Check
PLAT985_ALERT_1_G The Br-f"=    1.0411 Deviates from the B&C-Value    1.0006 Check
PLAT985_ALERT_1_G The Cu-f"=    3.6937 Deviates from the B&C-Value    3.6876 Check
PLAT985_ALERT_1_G The  F-f"=    0.0411 Deviates from the B&C-Value    0.0400 Check
PLAT985_ALERT_1_G The  P-f"=    0.3354 Deviates from the B&C-Value    0.3332 Check
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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
  10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  99 **ALERT level G** = General information/check it is not something unexpected

  18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
  67 ALERT type 4 Improvement, methodology, query or suggestion
   1 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_PLAT220_isn166_130k
;
PROBLEM: Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
RESPONSE: ...
;
_vrf_PLAT241_isn166_130k
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of       C10 Check
RESPONSE: ...
;
_vrf_PLAT260_isn166_130k
;
PROBLEM: Large Average Ueq of Residue Including        P3     0.106 Check
RESPONSE: ...
;
_vrf_PLAT329_isn166_130k
;
PROBLEM: Carbon Atom Hybridisation Unclear for ..........       C10 Check
RESPONSE: ...
;
_vrf_PLAT332_isn166_130k
;
PROBLEM: Large Phenyl C-C Range     C13        -C37       .      0.17 Ang.
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RESPONSE: ...
;
_vrf_PLAT341_isn166_130k
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............    0.00985 Ang.
RESPONSE: ...
;
_vrf_PLAT911_isn166_130k
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600        43 Report
RESPONSE: ...
;
_vrf_PLAT918_isn166_130k
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .        6 Check
RESPONSE: ...
;
_vrf_PLAT977_isn166_130k
;
PROBLEM: Check Negative Difference Density on H10          -0.34 eA-3
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 07/08/2019; check.def file version of 30/07/2019