checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2, 3, 4, 5

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

```
Bond precision:   C-C = 0.0020 A          Wavelength=1.54186

Cell:             a=7.2566(2)     b=37.7315(9)          c=8.4952(3)
                  alpha=90        beta=103.354(4)       gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           2263.12(12)               2263.11(12)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C48 H50 Cu F6 N6 O8       C48 H50 Cu F6 N6 O8
Sum formula      C48 H50 Cu F6 N6 O8       C48 H50 Cu F6 N6 O8
Mr               1016.49                   1016.50
Dx,g cm-3        1.492                     1.492
Z                2                         2
Mu (mm-1)        1.438                     1.438
F000             1054.0                    1054.1
F000'            1053.65
h,k,lmax         8,46,10                   8,46,10
Nref             4362                      4298
Tmin,Tmax        0.772,0.842
Tmin'            0.605

Correction method= Not given

Data completeness= 0.985           Theta(max)= 70.850

R(reflections)= 0.0283( 3591)                wR2(reflections)=
                                             0.0739( 4298)
S = 1.015                Npar= 413
```

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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.47 Report
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O1W      -H1WB      .      89.45 Degree
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C7       - H7A      .       1.12 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C9       - H9A      .       1.12 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C10      - H10A     .       1.14 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C10      - H10B     .       1.15 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C10      - H10C     .       1.15 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H14      ..H23      .       1.94 Ang.
                                                     x,y,z  =      1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         22 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.14 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............         3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        54 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         2 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        18 Info
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..............     Please Note
```

```
   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
  12 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Datablock: 2

```
Bond precision:   C-C = 0.0020 A          Wavelength=1.54186

Cell:             a=7.2566(2)     b=37.7315(9)          c=8.4952(3)
                  alpha=90        beta=103.354(4)       gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	2263.12(12)	2263.11(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H50 Cu F6 N6 O8	C48 H50 Cu F6 N6 O8
Sum formula	C48 H50 Cu F6 N6 O8	C48 H50 Cu F6 N6 O8
Mr	1016.49	1016.50
Dx,g cm-3	1.492	1.492
Z	2	2
Mu (mm-1)	1.438	1.438
F000	1054.0	1054.1
F000'	1053.65	
h,k,lmax	8,46,10	8,46,10
Nref	4362	4298
Tmin,Tmax		
Tmin'	0.605	

Correction method= Not given

Data completeness= 0.985 Theta(max)= 70.850

R(reflections)= 0.0283(3591) wR2(reflections)= 0.0739(4298)

S = 1.015 Npar= 413

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
greenish

Alert level G

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:C46 H44 Cu1 F6.029 N8 O6
Atom count from the _atom_site data: C46 H44 Cu1 F6.008 N8 O6

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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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 3

```
Bond precision:   C-C = 0.0011 A           Wavelength=1.54186

Cell:             a=7.9338(1)     b=10.2793(2)        c=28.5066(5)
                  alpha=90        beta=94.659(1)      gamma=90
Temperature:      100 K

                 Calculated                 Reported
Volume           2317.14(7)                 2317.14(7)
Space group      P 21/n                     P 1 21/n 1
Hall group       -P 2yn                     -P 2ybc (x-
Moiety formula   C48 H54 Cl2 Cu N6 O8       C48 H54 Cl2 Cu N6 O8
Sum formula      C48 H54 Cl2 Cu N6 O8       C48 H54 Cl2 Cu N6 O8
Mr               977.42                     977.45
Dx,g cm-3        1.401                      1.401
Z                2                          2
Mu (mm-1)        2.224                      2.224
F000             1022.0                     1022.7
F000'            1022.26
h,k,lmax         9,12,35                    9,12,34
Nref             4517                       4473
Tmin,Tmax        0.482,0.573                0.067,0.443
Tmin'            0.437

Correction method= # Reported T Limits: Tmin=0.067 Tmax=0.443
AbsCorr = MULTI-SCAN

Data completeness= 0.990           Theta(max)= 71.660

R(reflections)= 0.0191( 4148)                wR2(reflections)=
                                             0.0486( 4473)
S = 1.064                  Npar= 455
```

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

```
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................       9.83 Note
PLAT126_ALERT_1_C Error in or Uninterpretable Hall Symbol  ..... -P 2YBC (X Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O1W      -H1WA      .      87.94 Degree
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C8       - H8A      .       1.12 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         53 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         48 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         14 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C21      --C22      .        7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O1       .        9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O1W      .       14.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        46% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      11.80 Deg.
              C12A -C11  -C12     1_555   1_555   1_555 ......     #   70 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.13 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        112 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         41 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...          1 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..............     Please Note
```

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: 4

No errors found in this datablock

```
Bond precision:   C-C = 0.0011 A          Wavelength=1.54186

Cell:             a=7.9338(1)     b=10.2793(2)        c=28.5066(5)
                  alpha=90        beta=94.659(1)      gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	2317.14(7)	2317.14(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C48 H54 Cl2 Cu N6 O8	C48 H54 Cl2 Cu N6 O8
Sum formula	C48 H54 Cl2 Cu N6 O8	C48 H54 Cl2 Cu N6 O8
Mr	977.42	977.45
Dx,g cm-3	1.401	1.401
Z	2	2
Mu (mm-1)	2.224	2.224
F000	1022.0	1022.7
F000'	1022.26	
h,k,lmax	9,12,35	9,12,34
Nref	4517	4473
Tmin,Tmax		
Tmin'	0.437	

Correction method= Not given

Data completeness= 0.990 Theta(max)= 71.660

R(reflections)= 0.0191(4148) wR2(reflections)= 0.0486(4473)

S = 1.064 Npar= 455

Datablock: 5

Bond precision: C-C = 0.0017 A Wavelength=1.54186

Cell:	a=7.8787(1)	b=10.3607(3)	c=28.6114(5)
	alpha=90	beta=94.888(1)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	2327.02(8)	2327.02(8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C50 H60 Cu N6 O8	C50 H60 Cu N6 O8
Sum formula	C50 H60 Cu N6 O8	C50 H60 Cu N6 O8
Mr	936.59	936.61
Dx,g cm-3	1.337	1.337
Z	2	2
Mu (mm-1)	1.158	1.158
F000	990.0	989.2
F000'	988.86	
h,k,lmax	9,12,35	9,12,34
Nref	4554	4398
Tmin,Tmax	0.742,0.812	0.280,0.432
Tmin'	0.657	

Correction method= # Reported T Limits: Tmin=0.280 Tmax=0.432
AbsCorr = MULTI-SCAN

Data completeness= 0.966 Theta(max)= 71.730

R(reflections)= 0.0240(3940) wR2(reflections)= 0.0556(4398)

S = 1.073 Npar= 467

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

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.42 Note
PLAT126_ALERT_1_C Error in or Uninterpretable Hall Symbol ..... -P 2YBC (X Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O1W -H1WA . 85.38 Degree
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C7 - H7A . 1.15 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C7 - H7B . 1.11 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C8 - H8A . 1.12 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C8 - H8B . 1.12 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9B . 1.11 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C10 - H10A . 1.12 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.033 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 59 Report

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 52 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 30 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

```
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.        14 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C19      --C24      .        5.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O1       .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O1W      .        6.5 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        46% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      13.60 Deg.
              C12A -C11  -C12     1_555   1_555   1_555 ......     #   70 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.12 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       207 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        94 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        14 Info
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..............     Please 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
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 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 18/05/2022; check.def file version of 17/05/2022