checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound1

```
Bond precision:  C-C = 0.0028 A          Wavelength=0.71073

Cell:            a=21.7540(17)     b=10.8312(9)     c=9.4429(8)
                 alpha=90          beta=90          gamma=90
Temperature:     296 K
```

	Calculated	Reported
Volume	2225.0(3)	2225.0(3)
Space group	P n n a	P n n a
Hall group	-P 2a 2bc	-P 2a 2bc
Moiety formula	C22 H17 Cu N5 O8	C22 H17 Cu N5 O8
Sum formula	C22 H17 Cu N5 O8	C22 H17 Cu N5 O8
Mr	542.96	542.96
Dx,g cm-3	1.621	1.621
Z	4	4
Mu (mm-1)	1.043	1.043
F000	1108.0	1108.0
F000’	1109.79	
h,k,lmax	28,14,12	28,14,12
Nref	2751	2751
Tmin,Tmax	0.748,0.820	0.748,0.820
Tmin’	0.709	

```
Correction method= EMPIRICAL

Data completeness= 1.000          Theta(max)= 28.190

R(reflections)= 0.0308( 2169)     wR2(reflections)= 0.0876( 2751)

S = 1.040                 Npar= 165
```

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

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 empirical

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.86
PLAT193_ALERT_1_C Cell and Diffraction Temperatures differ by ....          3 Deg
```

Alert level G

```
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............        1
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1    --  O1      ..       15.2 su
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.20 Ratio
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Cu1     (II)          2.31
```

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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

Datablock: compound2

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=5.8014(6) b=20.224(2) c=17.9295(19)
       alpha=90 beta=93.394(2) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	2099.9(4)	2099.9(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H20 Cu N4 O7	C22 H20 Cu N4 O7
Sum formula	C22 H20 Cu N4 O7	C22 H20 Cu N4 O7
Mr	515.97	515.97
Dx,g cm-3	1.632	1.632
Z	4	4
Mu (mm-1)	1.096	1.096
F000	1060.0	1060.0
F000’	1061.75	
h,k,lmax	7,26,23	7,26,23
Nref	5230	5230
Tmin,Tmax	0.800,0.848	0.800,0.848
Tmin’	0.794	

Correction method= EMPIRICAL

Data completeness= 1.000 Theta(max)= 28.320

R(reflections)= 0.0350(3990) wR2(reflections)= 0.0864(5230)

S = 1.025 Npar= 307

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

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 empirical

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.971

PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O1W -H1WA 56.44 Deg.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?

PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 4

PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum .... ?

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- O1W .. 11.0 su

PLAT303_ALERT_2_G Full Occupancy H-Atom H1WA with # Connections 2.00

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 71
C9 -N1 -CU1 -N4 -37.60 1.70 1.555 1.555 1.555 4.765

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 72
C22 -N1 -CU1 -N4 139.20 1.60 1.555 1.555 1.555 4.765

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2

PLAT794_ALERT_5_G Note: Tentative Bond Valency for Cu1 (II) 2.04

PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis ..... 35 Times

---

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

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

Datablock: compound3

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell:	a=10.1381(9)	b=10.3036(9)	c=12.7118(11)
	alpha=80.201(2)	beta=71.420(1)	gamma=72.335(1)
Temperature:	296 K		

	Calculated	Reported
Volume	1195.33(18)	1195.33(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H17 Cu N4 O8, 2(H2 O)	C23 H22 Cu N4 O10
Sum formula	C23 H21 Cu N4 O10	C23 H22 Cu N4 O10
Mr	576.99	578.00
Dx,g cm-3	1.603	1.603
Z	2	2
Mu (mm-1)	0.981	0.981
F000	592.0	592.0
F000’	592.94	
h,k,lmax	12,12,15	12,12,15
Nref	4195	4195
Tmin,Tmax	0.783,0.830	0.783,0.830
Tmin’	0.783	

Correction method= EMPIRICAL

Data completeness= 1.000 Theta(max)= 24.990

R(reflections)= 0.0401(3626) wR2(reflections)= 0.1144(4173)

S = 1.087 Npar= 343

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

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 empirical
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.03
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 3.2 Ratio
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O .GT. 1.3 Ang) O4

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:C23 H22 Cu1 N4 O10
Atom count from the _atom_site data: C23 H21 Cu1 N4 O10
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?

```
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C23 H22 Cu N4 O10
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         46.00     46.00    0.00
           H         44.00     42.00    2.00
           Cu         2.00      2.00    0.00
           N          8.00      8.00    0.00
           O         20.00     20.00    0.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............        6
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         68
            C10 -N1  -CU1 -N4   -158.20  1.10   1.555   1.555   1.555   1.466
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         69
            C23 -N1  -CU1 -N4     22.80  1.30   1.555   1.555   1.555   1.466
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Cu1     (II)          2.16
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis .............         1 Times
```

---

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

   8 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
   0 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   5 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

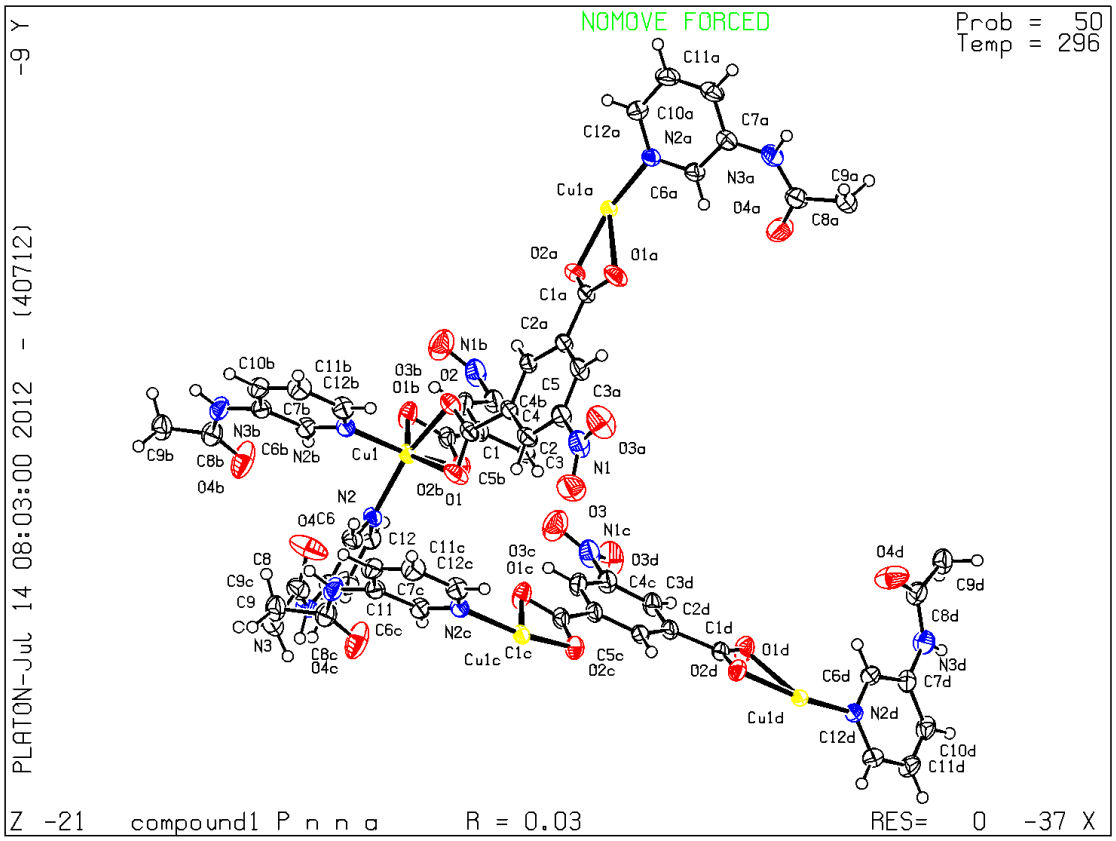
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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

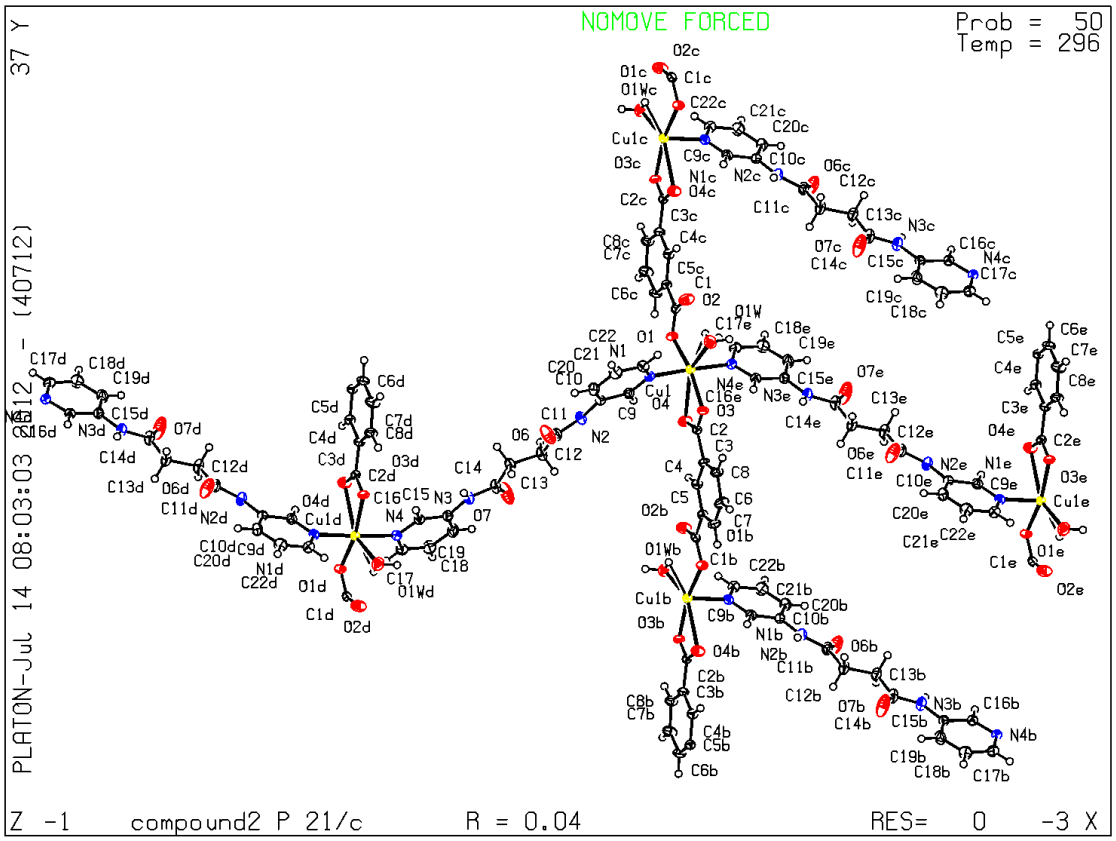
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 04/07/2012; check.def file version of 28/06/2012

Datablock compound1 - ellipsoid plot



Datablock compound2 - ellipsoid plot



Datablock compound3 - ellipsoid plot