checkCIF/PLATON report

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

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 = 0.0030 A Wavelength=0.71073

Cell: a=8.7640(5) b=9.4490(6) c=12.2731(5)
alpha=82.134(4) beta=83.863(4) gamma=75.190(5)
Temperature: 295 K

	Calculated	Reported
Volume	970.59(9)	970.59(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H28 Cu2 N10 O4 S4, 2(C N S), 2(C H4 O)	C22 H28 Cu2 N10 O4 S4, 2(C N S), 2(C H4 O)
Sum formula	C26 H36 Cu2 N12 O6 S6	C26 H36 Cu2 N12 O6 S6
Mr	932.13	932.13
Dx,g cm-3	1.595	1.595
Z	1	1
Mu (mm-1)	1.474	1.474
F000	478.0	478.0
F000’	479.50	
h,k,lmax	10,11,15	10,11,15
Nref	3960	3950
Tmin,Tmax	0.607,0.795	0.578,0.805
Tmin’	0.441	

Correction method= # Reported T Limits: Tmin=0.578 Tmax=0.805
AbsCorr = ANALYTICAL

Data completeness= 0.997 Theta(max)= 26.376

R(reflections)= 0.0286(3536) wR2(reflections)= 0.0730(3950)

S = 1.054 Npar= 252

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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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C12 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O3      0.089 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         7 Note
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S2       --C11      .        5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --N3       .        5.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --N5       .        5.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6E        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6F        Constrained at        0.5 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.37 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
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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
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   0 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
   3 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: 2

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

Cell: a=13.4682(4) b=12.6874(3) c=22.3679(4)
alpha=90 beta=90 gamma=90

Temperature: 295 K

	Calculated	Reported
Volume	3822.15(16)	3822.15(16)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C11 H14 Cu N5 O2 S2, N O3, C H4 O	C11 H14 Cu N5 O2 S2, N O3, C H4 O
Sum formula	C12 H18 Cu N6 O6 S2	C12 H18 Cu N6 O6 S2
Mr	469.99	469.98
Dx,g cm-3	1.633	1.633
Z	8	8
Mu (mm-1)	1.404	1.404
F000	1928.0	1928.0
F000’	1933.23	
h,k,lmax	16,15,27	16,15,27
Nref	3923	3909
Tmin,Tmax	0.454,0.726	0.546,0.739
Tmin’	0.445	

Correction method= # Reported T Limits: Tmin=0.546 Tmax=0.739
AbsCorr = ANALYTICAL

Data completeness= 0.996 Theta(max)= 26.404

R(reflections)= 0.0338(3442) wR2(reflections)= 0.0812(3909)

S = 1.148 Npar= 253

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

PLAT244_ALERT_4_C	Low	’Solvent’ Ueq as Compared to Neighbors of		N6	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		O6	0.083	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N1	--H1	.	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			4.589	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		2	Report

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			4	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension			1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms			3	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records			2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	S2	--C11 .	8.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	N5	--C11 .	5.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1	--N5 .	5.2	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A		Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B		Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6C		Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6D		Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6E		Constrained at	0.5	Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H6F        Constrained at        0.5 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.33 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          8 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
```

```
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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

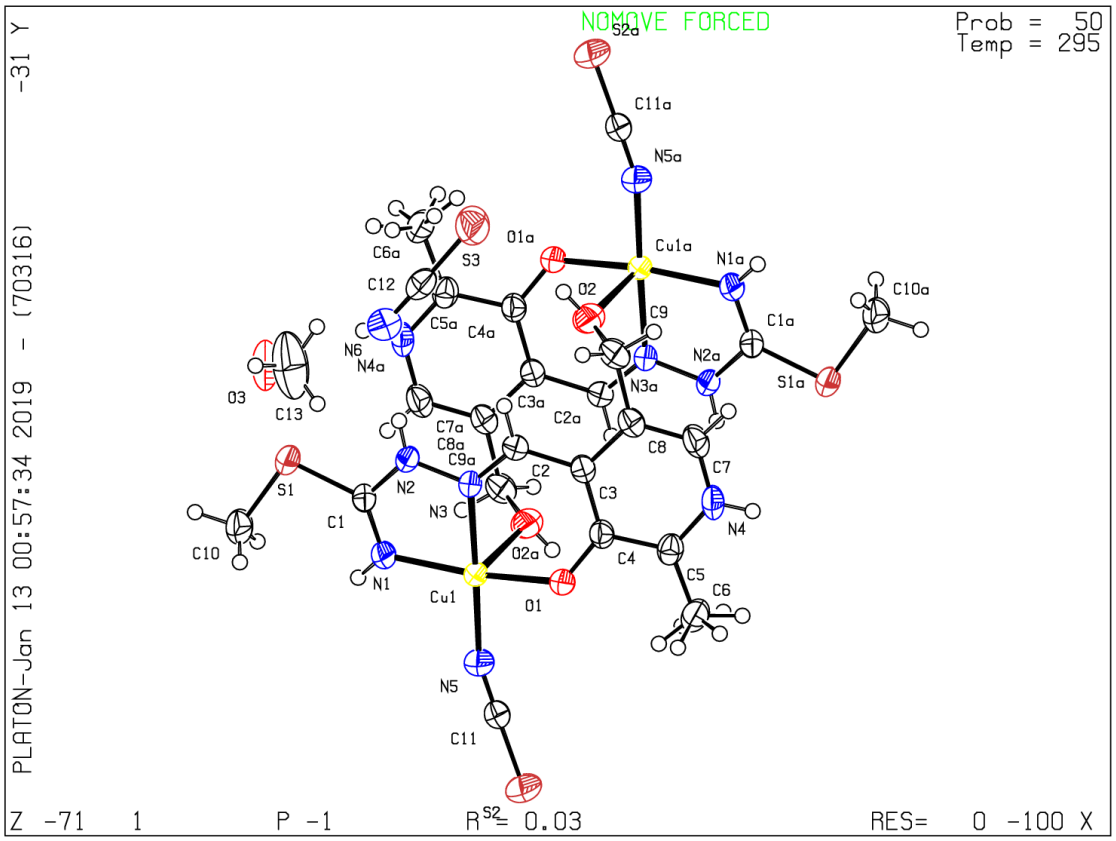
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 06/01/2019; check.def file version of 19/12/2018

Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot