

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 6

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: 6

Bond precision: C-C = 0.0025 A

Wavelength=0.71073

Cell: a=17.9524(17) b=11.0913(7) c=16.3512(15)
 alpha=90 beta=100.154(8) gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	3204.8(5)	3204.8(5)
Space group	I 2/a	I 1 2/a 1
Hall group	-I 2ya	-I 2ya
Moiety formula	C20 H34 Cu N4 O4 S2, 2(Cl O4)	C20 H34 Cu N4 O4 S2, 2(Cl O4)
Sum formula	C20 H34 Cl2 Cu N4 O12 S2	C20 H34 Cl2 Cu N4 O12 S2
Mr	721.08	721.07
Dx,g cm-3	1.495	1.494
Z	4	4
Mu (mm-1)	1.038	1.038
F000	1492.0	1492.0
F000'	1496.12	
h,k,lmax	22,13,20	22,13,20
Nref	3287	3287
Tmin,Tmax	0.799,0.949	0.644,1.000
Tmin'	0.583	

Correction method= # Reported T Limits: Tmin=0.644 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta(max)= 26.372

R(reflections)= 0.0340(2795)

wR2(reflections)= 0.0902(3287)

S = 1.035

Npar= 229

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

PLAT220_ALERT_2_C	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT222_ALERT_3_C	Non-Solv.	Resd 1	H	Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O2	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	S1	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N3	Check	
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	Cl1	Check	
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including			Cl1	0.132	Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group I2/a	I2/c	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	80%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C10	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	2.14	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	101	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
6 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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.

