

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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 = 0.0096 Å Wavelength=0.71073

Cell: a=18.770(6) b=13.876(4) c=19.169(6)
 alpha=90 beta=107.587(6) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	4759(3)	4759(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C48 H38 Cu N2 O P2, F6 P, C H2 Cl2	?
Sum formula	C49 H40 Cl2 Cu F6 N2 O P3	C49 H40 Cl2 Cu F6 N2 O P3
Mr	1014.19	1014.18
Dx, g cm ⁻³	1.416	1.415
Z	4	4
Mu (mm ⁻¹)	0.734	0.734
F000	2072.0	2072.0
F000'	2076.57	
h,k,lmax	22,16,22	22,16,22
Nref	8412	8403
Tmin,Tmax	0.753,0.802	0.851,0.886
Tmin'	0.738	

Correction method= # Reported T Limits: Tmin=0.851 Tmax=0.886
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.028

R(reflections)= 0.0654(5451) wR2(reflections)= 0.2000(8403)

S = 1.030 Npar= 596

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O1	--C12	.	7.0 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C27	--C48	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C29	--C41	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	P3	--F4	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	P3	--F5	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	P3	--F6	.	0.23 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O1			Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C23			Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C39			Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C44			Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C45			Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C48			Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C49			Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	P3			0.223 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl1			0.217 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds				0.0096 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				2.802 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595			9 Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.				0 Info

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				2 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				5.15 Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records				1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cul	--N1	.		5.7 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P3			Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6A	Constrained at			0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			2% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)				14% Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1				103.9 Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				6 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .				Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still				31% Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
- 0 **ALERT level B** = A potentially serious problem, consider carefully
- 19 **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
- 14 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
- 11 ALERT type 4 Improvement, methodology, query or suggestion
- 0 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.

