

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 = 0.0059 A	Wavelength=0.71073
Cell:	a=11.8354(19)	b=12.846(2) c=16.611(3)
	alpha=81.292(2)	beta=75.165(3) gamma=67.200(2)
Temperature:	296 K	
	Calculated	Reported
Volume	2246.7(6)	2246.6(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H39 Cu N3 P2, F6 P	?
Sum formula	C48 H39 Cu F6 N3 P3	C48 H39 Cu F6 N3 P3
Mr	928.28	928.27
Dx,g cm-3	1.372	1.372
Z	2	2
Mu (mm-1)	0.655	0.655
F000	952.0	952.0
F000'	953.66	
h,k,lmax	14,15,20	14,15,20
Nref	8372	8281
Tmin,Tmax	0.770,0.822	0.851,0.886
Tmin'	0.770	

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

Data completeness= 0.989 Theta(max)= 25.498

R(reflections)= 0.0426(6517) wR2(reflections)= 0.1276(8281)

S = 1.048 Npar= 550

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**

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C19	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C22	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C1	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	P4	0.137	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	84	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)	.	1	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1	--P1 .	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1	--P2 .	9.0	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P4	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F3	..C25	2.96	Ang.
		x,y,z =	1_555	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	7	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		9	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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
9 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

