checkCIF/PLATON report

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

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.

Datablock: as

Bond precision:	C-C = 0.0072 A	Wavelength=0.71073				
Cell:	a=11.7049(8) alpha=90		5 (12) 515 (2)	c=15.4895(15) gamma=90		
Temperature:	273 K					
Volume Space group Hall group	-		Reported 3152.4(4) I2/c -I2yc			
Moiety formula	C24 H20 Cu F6 N8	Si [+	?			
Sum formula	solvent] C24 H20 Cu F6 N8 solvent]	Si [+	C24 H20 C	u F6 N8 Si		
Mr	626.12		626.11			
Dx,g cm-3	1.319		1.319			
Z	4		4			
Mu (mm-1)	0.792		0.792			
F000	1268.0		1268.0			
F000'	1270.21		15 22 20			
h,k,lmax Nref	15,22,20 3645		15,22,20 3641			
Tmin, Tmax	0.888,0.909		3041			
Tmin'	0.888					
Correction method= Not given						
Data completenes	ss= 0.999	Theta(m	ax) = 27.53	1		
R(reflections)=	0.0757(2935)			wR2(reflections) = 0.2710(3641)		
S = 1.093	Npar= 1	184				

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 B PLAT242_ALERT_2_B Low

'MainMol' Ueq as Compared to Neighbors of Sil Check PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

Alert level C

PLAT052_ALERT_1_C Info or	n Absorption Correction Method Not	Given	Please Do !
PLAT084_ALERT_3_C High wF	R2 Value (i.e. > 0.25)		0.27 Report
PLAT241_ALERT_2_C High	'MainMol' Ueq as Compared to Neighbo	ors of	F1 Check
PLAT241_ALERT_2_C High	'MainMol' Ueq as Compared to Neighbo	rs of	C3 Check
PLAT341_ALERT_3_C Low Bor	nd Precision on C-C Bonds		0.00725 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms	22 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	3 Info
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records	1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)	273 Check
PLAT200_ALERT_1_G Reporteddiffrn_ambient_temperature (K)	273 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	448 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) .	2.19 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON	1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	305 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check

- 0 ALERT level A = Most likely a serious problem resolve or explain
- 2 ALERT level B = A potentially serious problem, consider carefully
- 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 14 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 5 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
- 5 ALERT type 4 Improvement, methodology, query or suggestion
- 3 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.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

