

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh073_sq

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: deh073_sq

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=24.0469(7) b=9.4323(3) c=20.6401(6)	
	alpha=90 beta=93.4900(16) gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	4672.9(2)	4672.9(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C52 H40 Cu N2 P2, F6 P [+ solvent]	?
Sum formula	C52 H40 Cu F6 N2 P3 [+ solvent]	C104 H80 Cu2 F12 N4 P6
Mr	963.32	1926.62
Dx, g cm ⁻³	1.369	1.369
Z	4	2
Mu (mm ⁻¹)	0.632	0.632
F000	1976.0	1976.0
F000'	1979.37	
h,k,lmax	34,13,29	34,13,29
Nref	7215	7202
Tmin,Tmax	0.934,0.951	0.692,0.746
Tmin'	0.838	

Correction method= # Reported T Limits: Tmin=0.692 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 30.614

R(reflections)= 0.0540(4808) wR2(reflections)= 0.1144(7202)

S = 1.012 Npar= 292

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	P2 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).		5 Note



Alert level G

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	2.00 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	11.31 Why ?
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	109 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	9 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
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock deh073_sq - ellipsoid plot

