

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0062 A	Wavelength=1.54180
Cell:	a=14.0474(11) b=17.4236(14) c=18.3028(13)	
	alpha=90 beta=109.786(2) gamma=90	
Temperature:	123 K	
	Calculated	Reported
Volume	4215.3(6)	4215.2(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C45 H41 Cu N O P2 S, F6 P	C45 H41 Cu1 F6 N1 O1 P3 S1
Sum formula	C45 H41 Cu F6 N O P3 S	C45 H41 Cu1 F6 N1 O1 P3 S1
Mr	914.31	914.35
Dx,g cm-3	1.441	1.441
Z	4	4
Mu (mm-1)	2.810	2.810
F000	1880.0	1880.0
F000'	1882.13	
h,k,lmax	17,21,22	17,20,22
Nref	8034	7650
Tmin,Tmax	0.651,0.656	0.570,0.660
Tmin'	0.591	

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.660
AbsCorr = MULTI-SCAN

Data completeness= 0.952 Theta(max)= 70.226

R(reflections)= 0.0743(7275) wR2(reflections)= 0.1728(7603)

S = 0.994 Npar= 541

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 34 Note

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.09 Report
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio 3.2 prolat
PLAT215_ALERT_3_C Disordered C7 has ADP max/min Ratio 3.1 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00617 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 140 Report

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 ... 71 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for C7 --C8 .. 5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cul --S1 . 5.3 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C44 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45 Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C53 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C54 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C55 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C56 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C57 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C58 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C46 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C47 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C48 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C49 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C50 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C51 Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H61 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H62 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H81 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H82 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H83 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H84 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H85 Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H86	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H91	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H92	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H93	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H94	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H95	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H96	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H411	Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H421	Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H431	Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H441	Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H451	Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H521	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H522	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H531	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H541	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H561	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H571	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H581	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H461	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H471	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H481	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H491	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H501	Constrained at	0.35	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		27%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C24 ..C47		3.14	Ang.
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found			Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		599	Note
PLAT882_ALERT_1_G	No Datum for _diffn_reflsv_unetI/netI			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		243	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		2	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked			! Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		4	Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
79 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
66 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT094_I
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      2.09 Report
RESPONSE: ...
;
_vrf_PLAT213_I
;
PROBLEM: Atom C8          has ADP max/min Ratio .....      3.2 prolat
RESPONSE: ...
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;
_vrf_PLAT215_I
;
PROBLEM: Disordered C7          has ADP max/min Ratio .....      3.1 Note
RESPONSE: ...
;
_vrf_PLAT220_I
;
PROBLEM: Non-Solvent Resd 1  C   Ueq(max)/Ueq(min) Range          4.0 Ratio
RESPONSE: ...
;
_vrf_PLAT341_I
;
PROBLEM: Low Bond Precision on  C-C Bonds .....                0.00617 Ang.
RESPONSE: ...
;
_vrf_PLAT911_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      140 Report
RESPONSE: ...
;
# end Validation Reply Form

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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 09/11/2017; check.def file version of 08/11/2017

