

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pfphcomplex\_130k\_0m

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: pfphcomplex\_130k\_0m

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Bond precision:    C-C = 0.0114 Å                      Wavelength=1.54178

Cell:                      a=11.1913(7)              b=11.1913(7)              c=39.724(3)  
                            alpha=90                      beta=90                      gamma=90

Temperature:              130 K

	Calculated	Reported
Volume	4975.2(7)	4975.2(7)
Space group	P 41 2 2	P 41 2 2
Hall group	P 4w 2c	P 4w 2c
Moiety formula	C52 H44 Cu N8, F6 P [+ solvent]	C52 H44 Cu N8, F6 P, 1[C4H10O1]
Sum formula	C52 H44 Cu F6 N8 P [+ solvent]	C56 H54 Cu F6 N8 O P
Mr	989.47	1063.58
Dx, g cm <sup>-3</sup>	1.321	1.420
Z	4	4
Mu (mm <sup>-1</sup> )	1.481	1.535
F000	2040.0	2208.0
F000'	2039.42	
h,k,lmax	13,13,48	13,13,46
Nref	4757[ 2842]	4642
Tmin,Tmax	0.772,0.807	0.613,0.753
Tmin'	0.701	

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 1.63/0.98                      Theta(max)= 70.215

R(reflections)= 0.0679( 4412)                      wR2(reflections)= 0.2035( 4642)

S = 1.031                                      Npar= 310

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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.

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### ● Alert level B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N4	--C21	.	8.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C8	--C9	.	14.6 s.u.
PLAT369_ALERT_2_B	Long C(sp2)-C(sp2) Bond	C8	- C12	.	1.58 Ang.
PLAT987_ALERT_1_B	The Flack x is >> 0 - Do a BASF/TWIN Refinement				Please Check

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### ● Alert level C

PLAT234_ALERT_4_C	Large Hirshfeld Difference	C21	--C26	.	0.16 Ang.
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of			C9	Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of			C18	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including			P1	0.164 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....				0.0114 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H12	..H22	.	1.98 Ang.
			x,y,z =		1_555 Check
PLAT411_ALERT_2_C	Short Inter H...H Contact	H18	..H18	.	2.14 Ang.
			x,-1-y,1/2-z =		6_545 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			4 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)				1 Check

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### ● Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.

Atom count from \_chemical\_formula\_sum: C56 H54 Cu1 F6 N8 O1 P1

Atom count from the \_atom\_site data: C52 H44 Cu1 F6 N8 P1

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 4

From the CIF: \_chemical\_formula\_sum C56 H54 Cu F6 N8 O P

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	224.00	208.00	16.00
H	216.00	176.00	40.00
Cu	4.00	4.00	0.00
F	24.00	24.00	0.00
N	32.00	32.00	0.00
O	4.00	0.00	4.00
P	4.00	4.00	0.00

PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF .....	Please Check
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.057 Note
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	3.49 %
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12 Report
PLAT244_ALERT_4_G	Low Solvent Ueq as Compared to Neighbors of	P1 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	125 A**3
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	38 Note
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	2 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ	2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1 Check

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

8 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  
 6 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

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## 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_PLAT234_pfphcomplex_130k_0m
;
PROBLEM: Large Hirshfeld Difference C21      --C26      .      0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT241_pfphcomplex_130k_0m
;
PROBLEM: High      MainMol Ueq as Compared to Neighbors of      C9 Check
RESPONSE: ...
;
_vrf_PLAT260_pfphcomplex_130k_0m
;
PROBLEM: Large Average Ueq of Residue Including      P1      0.164 Check
RESPONSE: ...
;
_vrf_PLAT341_pfphcomplex_130k_0m
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.0114 Ang.
RESPONSE: ...
;
_vrf_PLAT410_pfphcomplex_130k_0m
;
PROBLEM: Short Intra H...H Contact  H12      ..H22      .      1.98 Ang.
RESPONSE: ...
;
_vrf_PLAT411_pfphcomplex_130k_0m
;
PROBLEM: Short Inter H...H Contact  H18      ..H18      .      2.14 Ang.
RESPONSE: ...
;
_vrf_PLAT911_pfphcomplex_130k_0m
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      4 Report
RESPONSE: ...
;
_vrf_PLAT918_pfphcomplex_130k_0m
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .      1 Check
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.

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**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

