

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.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: s2519lm

Bond precision: C-C = 0.0081 Å Wavelength=0.71073

Cell: a=9.8687(8) b=27.521(2) c=21.7494(17)
 alpha=90 beta=95.369(2) gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	5881.2(8)	5881.2(8)
Space group	P 21/c	P 21/c
Hall group	: -P 2ybc	-P 2ybc
Moiety formula	C64 H47 Br Cu N4 O P2, F6 P, C H2 Cl2	C64 H47 Br Cu N4 O P2, F6 P, C H2 Cl2
Sum formula	C65 H49 Br Cl2 Cu F6 N4 O P3	C65 H49 Br Cl2 Cu F6 N4 O P3
Mr	1323.35	1323.34
Dx, g cm ⁻³	1.495	1.495
Z	4	4
Mu (mm ⁻¹)	1.290	1.290
F000	2688.0	2688.0
F000'	2691.59	
h,k,lmax	11,32,25	11,32,25
Nref	10449	10384
Tmin,Tmax	0.926,0.938	0.628,0.745
Tmin'	0.753	

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.070

R(reflections)= 0.0700(4992) wR2(reflections)= 0.1047(10384)

S = 1.036 Npar= 751

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

```
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
                  Rint given    0.144
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..      48% Check
PLAT213_ALERT_2_C Atom C50          has ADP max/min Ratio .....      3.1 prolat
PLAT244_ALERT_4_C Low      'Solvent' Ueq as Compared to Neighbors of      C1X Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      C11X      0.100 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds .....      0.00814 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      38 Ang**3
```



Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF      Please Do !
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .....      0.144 Report
PLAT244_ALERT_4_G Low      'Solvent' Ueq as Compared to Neighbors of      P3 Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C4      -C11      .      1.42 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      2 Note
PLAT899_ALERT_4_G SHELXL97      is Deprecated and Succeeded by SHELXL      2018 Note
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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
7 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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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_RINTA01_s2519lm
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT026_s2519lm
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low ..      48% Check
RESPONSE: ...
;
_vrf_PLAT213_s2519lm
;
PROBLEM: Atom C50          has ADP max/min Ratio .....      3.1 prolat
RESPONSE: ...
;
_vrf_PLAT244_s2519lm
;
PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of      C1X Check
RESPONSE: ...
```

```

;
_vrf_PLAT260_s2519lm
;
PROBLEM: Large Average Ueq of Residue Including      Cl1X      0.100 Check
RESPONSE: ...
;
_vrf_PLAT341_s2519lm
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00814 Ang.
RESPONSE: ...
;
_vrf_PLAT601_s2519lm
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of .      38 Ang**3
RESPONSE: ...
;
# end Validation Reply Form

```

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 19/10/2018; check.def file version of 15/10/2018

