

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: cu_140630c_0m

Bond precision: C-C = 0.0020 A Wavelength=1.54178

Cell: a=14.8444(2) b=10.0477(2) c=8.0559(1)
 alpha=90 beta=91.023(1) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1201.36(3)	1201.36(3)
Space group	P c	P c
Hall group	P -2yc	P -2yc
Moiety formula	C24 H32 O8	C24 H32 O8
Sum formula	C24 H32 O8	C24 H32 O8
Mr	448.50	448.50
Dx,g cm-3	1.240	1.240
Z	2	2
Mu (mm-1)	0.768	0.768
F000	480.0	480.0
F000'	481.61	
h,k,lmax	18,12,9	17,11,9
Nref	4626[2319]	3951
Tmin,Tmax	0.891,0.912	0.894,0.914
Tmin'	0.891	

Correction method= # Reported T Limits: Tmin=0.894 Tmax=0.914
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.85 Theta(max)= 70.980

R(reflections)= 0.0334(3889) wR2(reflections)= 0.0911(3951)

S = 1.048 Npar= 297

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

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low 0.951 Note

Alert level C

PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 32 Ang3

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
PLAT792_ALERT_1_G The Model has Chirality at C7 (Polar SPGR) S Verify
PLAT792_ALERT_1_G The Model has Chirality at C7' (Polar SPGR) R Verify
PLAT792_ALERT_1_G The Model has Chirality at C8 (Polar SPGR) R Verify
PLAT792_ALERT_1_G The Model has Chirality at C8' (Polar SPGR) R Verify
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
2 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_PLAT601_cu_140630c_0m
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of . 32 Ang3
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*, 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 21/06/2015; check.def file version of 21/06/2015

