

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0097 A Wavelength=0.71073

Cell: a=34.1570(11) b=8.5558(3) c=19.8431(8)
 alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	5799.0(4)	5799.0(4)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C24 H37 B Ru2 S6	?
Sum formula	C24 H37 B Ru2 S6	C24 H37 B Ru2 S6
Mr	730.85	730.84
Dx,g cm-3	1.674	1.674
Z	8	8
Mu (mm-1)	1.487	1.487
F000	2960.0	2960.0
F000'	2946.28	
h,k,lmax	40,10,23	40,10,23
Nref	5055	5022
Tmin,Tmax	0.696,0.862	0.696,0.862
Tmin'	0.683	

Correction method= # Reported T Limits: Tmin=0.696 Tmax=0.862
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 24.930

R(reflections)= 0.0456(3085) wR2(reflections)= 0.0855(5022)

S = 0.993 Npar= 309

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**

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0097 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.593 30 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

● **Alert level G**

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 14.94 Why ?
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C8 Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 31% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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_PLAT342_shelx
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.0097 Ang.
RESPONSE: ...
;
_vrf_PLAT911_shelx
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.593 30 Report
RESPONSE: ...
;
_vrf_PLAT978_shelx
;
PROBLEM: Number C-C Bonds with Positive Residual Density. 0 Info
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 06/01/2019; check.def file version of 19/12/2018

