

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: shelxl

Bond precision: C-C = 0.0149 A Wavelength=0.71070

Cell: a=9.746(6) b=10.127(5) c=10.340(6)
 alpha=98.363(9) beta=111.609(15) gamma=91.830(18)

Temperature: 295 K

	Calculated	Reported
Volume	934.7(9)	934.7(9)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C19 H14 O3 P Re S2	C19 H14 O3 P Re S2
Sum formula	C19 H14 O3 P Re S2	C19 H14 O3 P Re S2
Mr	571.60	571.59
Dx,g cm-3	2.031	2.031
Z	2	2
Mu (mm-1)	6.825	6.826
F000	548.0	548.0
F000'	546.93	
h,k,lmax	12,13,13	12,12,12
Nref	4263	3359
Tmin,Tmax	0.180,0.293	0.055,0.068
Tmin'	0.069	

Correction method= # Reported T Limits: Tmin=0.055 Tmax=0.068
AbsCorr = MULTI SCAN

Data completeness= 0.788 Theta(max)= 27.430

R(reflections)= 0.0463(3084) wR2(reflections)= 0.1202(3359)

S = 1.071 Npar= 235

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 _diffn_measured_fraction_theta_full value Low . 0.948 Note

Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01487 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C4 - C5 .. 1.43 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus P1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 80 Note
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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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 08/07/2016; check.def file version of 05/07/2016

