

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: VG-16-042B

Bond precision: C-C = 0.0083 Å Wavelength=1.54184

Cell: a=10.5494(5) b=11.5375(6) c=21.871(1)
 alpha=76.877(4) beta=82.084(4) gamma=85.941(4)
Temperature: 173 K

	Calculated	Reported
Volume	2565.6(2)	2565.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H48 F3 N2 O P3 Ru Si, C H Cl3	C52 H48 F3 N2 O P3 Ru Si, C H Cl3
Sum formula	C53 H49 Cl3 F3 N2 O P3 Ru Si	C53 H49 Cl3 F3 N2 O P3 Ru Si
Mr	1115.36	1115.42
Dx, g cm ⁻³	1.444	1.444
Z	2	2
Mu (mm ⁻¹)	5.439	5.439
F000	1140.0	1147.4
F000'	1147.13	
h,k,lmax	12,14,26	12,14,26
Nref	10037	9464
Tmin,Tmax	0.509,0.762	0.397,1.000
Tmin'	0.385	

Correction method= # Reported T Limits: Tmin=0.397 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.943 Theta(max)= 71.740

R(reflections)= 0.0567(8126) wR2(reflections)= 0.1894(9464)

S = 1.303 Npar= 607

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 value Low . 0.943 Note

Author Response: a software glitch prevented collectino to 100%

PLAT230_ALERT_2_B Hirshfeld Test Diff for N1 -- C5 .. 8.3 s.u.

 **Alert level C**

PLAT213_ALERT_2_C Atom F3 has ADP max/min Ratio 3.3 prolat
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C01V Check
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00834 Ang.

 **Alert level G**

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
 PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
 PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- C2 .. 7.5 s.u.
 PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C01U Check
 PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus P1 Check
 PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C1 Check
 PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 .. O1 .. 3.12 Ang.
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
 PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
 C H Cl3
 PLAT982_ALERT_1_G The C-f' = 0.019 Deviates from the IT-value 0.018 Check
 PLAT982_ALERT_1_G The Cl-f' = 0.368 Deviates from the IT-value 0.364 Check
 PLAT982_ALERT_1_G The F-f' = 0.075 Deviates from the IT-value 0.073 Check
 PLAT982_ALERT_1_G The N-f' = 0.033 Deviates from the IT-value 0.031 Check
 PLAT982_ALERT_1_G The O-f' = 0.052 Deviates from the IT-value 0.049 Check
 PLAT982_ALERT_1_G The P-f' = 0.304 Deviates from the IT-value 0.296 Check
 PLAT982_ALERT_1_G The Ru-f' = 0.075 Deviates from the IT-value 0.055 Check
 PLAT982_ALERT_1_G The Si-f' = 0.255 Deviates from the IT-value 0.254 Check
 PLAT983_ALERT_1_G The Ru-f" = 3.268 Deviates from the IT-Value 3.296 Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 2 **ALERT level B** = A potentially serious problem, consider carefully
 - 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 20 **ALERT level G** = General information/check it is not something unexpected
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- 11 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
 - 2 ALERT type 3 Indicator that the structure quality may be low
 - 6 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_PLAT230_VG-16-042B
;
PROBLEM: Hirshfeld Test Diff for    N1      --  C5      ..      8.3 s.u.
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 11/08/2016; check.def file version of 04/08/2016

