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: JJJ

Bond precision: C-C = 0.0213 A Wavelength=0.71073

Cell: a=13.425(3) b=11.817(2) c=15.660(3)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2484.4(8)	2484.4(9)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C12 H24 O6, C6 H6 F2 N, F6 P	?
Sum formula	C18 H30 F8 N O6 P	C18 H30 F8 N O6 P
Mr	539.40	539.40
Dx,g cm-3	1.442	1.442
Z	4	4
Mu (mm-1)	0.203	0.203
F000	1120.0	1120.0
F000’	1121.35	
h,k,lmax	17,15,20	17,15,20
Nref	5697[2954]	5528
Tmin,Tmax		0.730,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.730 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.87/0.97 Theta(max)= 27.467

R(reflections)= 0.1370(3147) wR2(reflections)= 0.2955(5528)

S = 1.208 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 B

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02125 Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.14 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report
PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio ..... 3.7 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference O3 --C23 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20 --C24 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C3 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1 -C6 1.37 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C7 - C8 . 1.34 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H7A ..H8A 1.98 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H7B ..H8B 1.98 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.400 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 14 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  20 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
   8 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_ABSTY02_JJJ
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT053_JJJ
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT054_JJJ
;
PROBLEM: Medium  Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT055_JJJ
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT082_JJJ
;
PROBLEM: High R1 Value ..................................       0.14 Report
RESPONSE: ...
;
_vrf_PLAT084_JJJ
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.30 Report
RESPONSE: ...
;
_vrf_PLAT213_JJJ
;
PROBLEM: Atom C7              has ADP max/min Ratio .....        3.7 prolat
RESPONSE: ...
;
_vrf_PLAT234_JJJ
;
PROBLEM: Large Hirshfeld Difference O3       --C23             0.21 Ang.
RESPONSE: ...
;
_vrf_PLAT241_JJJ
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of        C11 Check
RESPONSE: ...
;
_vrf_PLAT242_JJJ
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         O1 Check
RESPONSE: ...
;
```

```
_vrf_PLAT244_JJJ
;
PROBLEM: Low    'Solvent' Ueq as Compared to Neighbors of         C3 Check
RESPONSE: ...
;
_vrf_PLAT250_JJJ
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
RESPONSE: ...
;
_vrf_PLAT334_JJJ
;
PROBLEM: Small Aver. Benzene C-C Dist C1       -C6             1.37 Ang.
RESPONSE: ...
;
_vrf_PLAT360_JJJ
;
PROBLEM: Short  C(sp3)-C(sp3) Bond  C7       - C8       .       1.34 Ang.
RESPONSE: ...
;
_vrf_PLAT410_JJJ
;
PROBLEM: Short Intra H...H Contact  H7A      ..H8A             1.98 Ang.
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 23/04/2018; check.def file version of 23/04/2018

Datablock JJJ - ellipsoid plot