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: 1

Bond precision: C-C = 0.0168 A Wavelength=0.71073

Cell: a=11.9791(10) b=13.6041(12) c=15.4202(8)
alpha=90 beta=90 gamma=90
Temperature: 323 K

	Calculated	Reported
Volume	2513.0(3)	2513.0(3)
Space group	C m c 21	C m c 21
Hall group	C 2c -2	C 2c -2
Moiety formula	C12 H24 O6, C6 H5 F2 N, F6 P	?
Sum formula	C18 H29 F8 N O6 P	C18 H30 F8 N O6 P
Mr	538.39	539.40
Dx,g cm-3	1.423	1.423
Z	4	4
Mu (mm-1)	0.201	0.201
F000	1116.0	1116.0
F000’	1117.35	
h,k,lmax	17,20,22	17,19,20
Nref	4401[2275]	3219
Tmin,Tmax	0.955,0.961	0.128,1.000
Tmin’	0.955	

Correction method= # Reported T Limits: Tmin=0.128 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.41/0.73 Theta(max)= 31.569

R(reflections)= 0.1896(1336) wR2(reflections)= 0.4942(3219)

S = 1.536 Npar= 244

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 A

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.49 Report

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Alert level B

PLAT082_ALERT_2_B High R1 Value ..... 0.19 Report
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01675 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
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 1.01 Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C3 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F5 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F6 0.20 Ang.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C4 Check
PLAT411_ALERT_2_C Short Inter H...H Contact H2A ..H12B 2.06 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C18 H30 F8 N1 O6 P1
Atom count from the _atom_site data: C18 H29 F8 N1 O6 P1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C18 H30 F8 N O6 P
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	72.00	72.00	0.00
H	120.00	116.00	4.00
F	32.00	32.00	0.00
N	4.00	4.00	0.00
O	24.00	24.00	0.00
P	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 30 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 28 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 10 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C1 --C2 . 5.7 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1C        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        11% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1            105.4 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2            102.8 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O3            106.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O4            108.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O5            103.7 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O6            104.7 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F5       ..C7              2.90 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         42 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       326 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ          2 Units
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully

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 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 74 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 60 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
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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.

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_1
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT084_1
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.49 Report
RESPONSE: ...
;
_vrf_PLAT026_1
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low ..        42% Check
RESPONSE: ...
;
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_vrf_PLAT041_1
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT043_1
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       1.01 Check
RESPONSE: ...
;
_vrf_PLAT234_1
;
PROBLEM: Large Hirshfeld Difference C2       --C3               0.17 Ang.
RESPONSE: ...
;
_vrf_PLAT244_1
;
PROBLEM: Low    'Solvent' Ueq as Compared to Neighbors of         C1 Check
RESPONSE: ...
;
_vrf_PLAT411_1
;
PROBLEM: Short Inter H...H Contact  H2A      ..H12B             2.06 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock 1 - ellipsoid plot