checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: 40msbm

Bond precision: C-C = 0.0139 A Wavelength=0.71073

Cell: **a=32.186(4)** **b=11.5459(13)** **c=12.7286(15)**
alpha=90 **beta=104.996(3)** **gamma=90**
Temperature: **298 K**

	Calculated	Reported
Volume	4569.1(9)	4569.1(9)
Space group	C 2/m	C2/m
Hall group	-C 2y	?
Moiety formula	C14 H11 O6, C16 H14 O4, C8 H3 N2, F6 P	?
Sum formula	C38 H28 F6 N2 O10 P	C39 H44 F6 N2 O10 P
Mr	817.59	845.73
Dx,g cm-3	1.189	1.229
Z	4	4
Mu (mm-1)	0.135	0.136
F000	1676.0	1764.0
F000’	1677.58	
h,k,lmax	38,13,15	38,13,15
Nref	4249	4223
Tmin,Tmax	0.993,0.997	0.981,0.997
Tmin’	0.981	

Correction method= MULTI-SCAN

Data completeness= 0.994 **Theta(max)= 25.000**

R(reflections)= 0.1828(2412) **wR2(reflections)= 0.4747(4223)**

S = 1.493 **Npar= 266**

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

RFACR01_ALERT_3_A The value of the weighted R factor is > 0.45
Weighted R factor given 0.475
SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 1.068
Additional refinement cycles may be required.

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PLAT080_ALERT_2_A Maximum Shift/Error ..........................      1.07
PLAT084_ALERT_2_A High wR2 Value ...............................      0.47
PLAT213_ALERT_2_A Atom C22            has ADP max/min Ratio .....      5.10 oblat
PLAT220_ALERT_2_A Large Non-Solvent    C     Ueq(max)/Ueq(min) ...      9.63 Ratio
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for       C20
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .    333.00 A**3
PLAT093_ALERT_1_A No su's on H-atoms, but refinement reported as .     mixed
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Alert level B

```
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      1.909
           Test value =      1.500
RFACG01_ALERT_3_B  The value of the R factor is > 0.15
           R factor given   0.183
PLAT082_ALERT_2_B High R1 Value ................................      0.18
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density      1.91 eA-3
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......         4
PLAT213_ALERT_2_B Atom C24            has ADP max/min Ratio .....      4.30 oblat
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...      4.18 Ratio
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...      4.42 Ratio
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       O9
PLAT326_ALERT_2_B Check for Possibly Missing H on sp3? Carbon ....     <C11B
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds (x 1000) Ang ..       14
PLAT430_ALERT_2_B Short Inter D...A Contact  O9     ..  O12     ..      2.78 Ang.
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Alert level C

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CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.99 <> 1.01
          From the CIF: _cell_formula_units_Z                  4
          From the CIF: _chemical_formula_weight          845.73
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          C        12.01   38.00  456.42
          F        19.00    6.00  113.99
          P        30.97    1.00   30.97
          O        16.00   10.00  159.99
          H         1.01   28.00   28.22
          N        14.01    2.00   28.01
          Calculated formula weight            817.61
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       O12
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C14
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       O15
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C13
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C18
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C30
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      3.49
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.58
PLAT313_ALERT_2_C Oxygen with three covalent bonds (rare) ........       O19
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C24    -   C25    ...      1.38 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ         ?
PLAT043_ALERT_1_C Check Reported Molecular Weight ................    845.73
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...         ?
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....         ?
PLAT231_ALERT_4_C Hirshfeld Test (Solvent)   P1     --  F3      ..      5.65 su
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PLAT234_ALERT_4_C Large Hirshfeld Difference O15    --  C14     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C16    --  C17     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F4      ..       0.15 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1
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Alert level G

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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:C39 H44 F6 N2 O10 P1
           Atom count from the _atom_site data:  C38 H28 F6 N2 O10 P1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C39 H44 F6 N2 O10 P
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        156.00    152.00    4.00
           H        176.00    112.00   64.00
           F         24.00     24.00    0.00
           N          8.00      8.00    0.00
           O         40.00     40.00    0.00
           P          4.00      4.00    0.00
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      18.00 Perc.
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C24
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C25
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C27
PLAT432_ALERT_2_G Short Inter X...Y Contact  O9     ..  C11B    ..       2.38 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O9     ..  C11A    ..       2.47 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O12    ..  C10A    ..       2.28 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O12    ..  C10B    ..       2.49 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C11A   ..  C10A    ..       1.55 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C10B   --  C11A    .        2.04 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C30    --  C30     .        1.96 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          7
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         47
             O12  -C11B -C11A    1.555   1.555   1.555             38.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         64
             C20  -C19  -O21     1.555   1.555   1.555             38.90 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
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   9 ALERT level A = In general: serious problem
  12 ALERT level B = Potentially serious problem
  24 ALERT level C = Check and explain
  20 ALERT level G = General alerts; check

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  40 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
   9 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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*, 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 22/10/2010; check.def file version of 11/10/2010

Datablock 40msbm - ellipsoid plot