checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound2

```
Bond precision:  C-C = 0.0103 A          Wavelength=0.71073

Cell:             a=10.830(2)     b=16.351(3)        c=18.379(4)
                  alpha=90        beta=99.45(3)      gamma=90
Temperature:      293 K
```

	Calculated	Reported
Volume	3210.4(11)	3210.3(11)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C30 H28 Cl N8 Ru, F6 P	?
Sum formula	C30 H28 Cl F6 N8 P Ru	C30 H28 Cl F6 N8 P Ru
Mr	782.09	782.09
Dx,g cm-3	1.618	1.618
Z	4	4
Mu (mm-1)	0.692	0.692
F000	1576.0	1576.0
F000’	1572.66	
h,k,lmax	12,18,21	12,18,21
Nref	5186	4993
Tmin,Tmax	0.883,0.940	0.840,0.928
Tmin’	0.824	

```
Correction method= MULTI-SCAN

Data completeness= 0.963          Theta(max)= 24.230

R(reflections)= 0.0530( 1457)     wR2(reflections)= 0.0878( 4993)

S = 0.600                 Npar= 364
```

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

```
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   5.831
           Additional refinement cycles may be required.
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections too Low ....        29 Perc.
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PLAT073_ALERT_1_A H-atoms ref, but _hydrogen_treatment reported as     constr
PLAT080_ALERT_2_A Maximum Shift/Error ..........................       5.83
PLAT211_ALERT_2_A ADP of Atom C9      is N.P.D. or (nearly) 2D ...          ?
PLAT213_ALERT_2_A Atom N2              has ADP max/min Ratio .....        6.5 prola
```

Alert level B

```
RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
           Rint given   0.192
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        8.7 Ratio
PLAT222_ALERT_3_B Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        8.4 Ratio
```

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
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.600
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5774
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.962
PLAT166_ALERT_4_C S.U's Given on Coordinates for calc-flagged ....        H27
PLAT213_ALERT_2_C Atom N5              has ADP max/min Ratio .....        3.3 prola
PLAT213_ALERT_2_C Atom N7              has ADP max/min Ratio .....        3.4 oblat
PLAT213_ALERT_2_C Atom C2              has ADP max/min Ratio .....        3.3 prola
PLAT213_ALERT_2_C Atom C19             has ADP max/min Ratio .....        3.5 prola
PLAT213_ALERT_2_C Atom C23             has ADP max/min Ratio .....        3.4 prola
PLAT213_ALERT_2_C Atom C28             has ADP max/min Ratio .....        3.3 prola
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  N3      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  C6      ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C11     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6     --  N7      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5     --  C6      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9     --  C10     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17    --  C18     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21    --  C26     ..       0.17 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C4
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C20
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C27
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          P
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0103 Ang
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C27    -   C28    ...       1.40 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         69 A**3
PLAT732_ALERT_1_C Angle   Calc     37.3(3), Rep   37.30(10) ......       3.00 su-Ra
             C23  -RU   -C24     1.555   1.555   1.555      #          6
PLAT732_ALERT_1_C Angle   Calc     37.3(3), Rep   37.29(10) ......       3.00 su-Ra
             C23  -RU   -C22     1.555   1.555   1.555      #          9
PLAT732_ALERT_1_C Angle   Calc     67.2(3), Rep   67.20(13) ......       2.31 su-Ra
             C24  -RU   -C22     1.555   1.555   1.555      #         10
PLAT732_ALERT_1_C Angle   Calc     37.2(3), Rep   37.23(11) ......       2.73 su-Ra
             C24  -RU   -C25     1.555   1.555   1.555      #         14
PLAT732_ALERT_1_C Angle   Calc     79.3(3), Rep   79.30(14) ......       2.14 su-Ra
             C22  -RU   -C25     1.555   1.555   1.555      #         15
PLAT732_ALERT_1_C Angle   Calc     79.3(3), Rep   79.30(14) ......       2.14 su-Ra
             C24  -RU   -C21     1.555   1.555   1.555      #         19
PLAT732_ALERT_1_C Angle   Calc     37.2(3), Rep   37.13(11) ......       2.73 su-Ra
             C25  -RU   -C26     1.555   1.555   1.555      #         27
```

```
PLAT732_ALERT_1_C Angle   Calc     37.1(3), Rep   37.12(10) ......       3.00 su-Ra
             C21  -RU   -C26     1.555   1.555   1.555      #         28
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          1
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
```

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

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  12 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*, 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 28/03/2012; check.def file version of 18/03/2012

Datablock compound2 - ellipsoid plot