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: compund7

```
Bond precision:  C-C = 0.0113 A          Wavelength=0.71073

Cell:           a=8.4962(17)      b=10.542(2)      c=18.076(4)
                alpha=85.91(3)    beta=82.53(3)    gamma=83.89(3)
Temperature:    293 K
```

	Calculated	Reported
Volume	1593.4(6)	1593.5(6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H29 Cl N8 Rh, F6 P	?
Sum formula	C30 H29 Cl F6 N8 P Rh	C30 H29 Cl F6 N8 P Rh
Mr	784.94	784.94
Dx,g cm-3	1.636	0.818
Z	2	2
Mu (mm-1)	0.741	0.371
F000	792.0	792.0
F000’	790.62	
h,k,lmax	9,11,19	9,11,19
Nref	4299	4047
Tmin,Tmax	0.938,0.956	0.830,0.890
Tmin’	0.921	

```
Correction method= MULTI-SCAN

Data completeness= 0.941          Theta(max)= 22.730

R(reflections)= 0.0372( 1771)     wR2(reflections)= 0.0543( 4047)

S = 0.486                 Npar= 429
```

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

```
ABSMU01_ALERT_1_A  The ratio of given/expected absorption coefficient lies
              outside the range 0.90 <> 1.10
           Calculated value of mu =     0.741
           Value of mu given      =     0.371
```

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DENSD01_ALERT_1_A  The ratio of the submitted crystal density and that
           calculated from the formula is outside the range 0.90 <> 1.10
           Crystal density given    =      0.818
           Calculated crystal density =      1.636
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.5437
PLAT046_ALERT_1_A Reported Z, MW and D(calc) are Inconsistent ....      1.636
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      99.84 Perc.
```

Alert level B

```
GOODF01_ALERT_2_B  The least squares goodness of fit parameter lies
           outside the range 0.60 <> 4.00
           Goodness of fit given =      0.486
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low .......      0.942
PLAT214_ALERT_2_B Atom F5      (Anion/Solvent) ADP max/min Ratio          5.7 prola
```

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
REFLT03_ALERT_3_C  Reflection count < 95% complete
          From the CIF: _diffrn_reflns_theta_max          22.73
          From the CIF: _diffrn_reflns_theta_full         22.73
          From the CIF: _reflns_number_total              4047
          TEST2: Reflns within _diffrn_reflns_theta_max
          Count of symmetry unique reflns         4299
          Completeness (_total/calc)            94.14%
REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
           centrosymmetric structure
           sine(theta)/lambda               0.5437
           Proportion of unique data used   1.0000
           Ratio reflections to parameters  9.4336
PLAT022_ALERT_3_C Ratio Unique / Expected Reflections (too) Low ..      0.941
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         44 Perc.
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................       9.43
PLAT213_ALERT_2_C Atom C22            has ADP max/min Ratio .....        3.2 prola
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        3.7 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        4.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N8     --  C20     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21    --  C22     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P      --  F5      ..       0.22 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          P
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0113 Ang
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....         ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.03000 Deg.
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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   5 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected
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  9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  4 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 compund7 - ellipsoid plot