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: CompoundI

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

Cell:           a=28.5598(19)    b=14.0774(9)      c=10.7417(6)
                alpha=90         beta=91.123(3)    gamma=90
Temperature:    120 K
```

	Calculated	Reported
Volume	4317.9(5)	4317.8(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C46 H28 Co4 N6 O15	C46 H28 Co4 N6 O15
Sum formula	C46 H28 Co4 N6 O15	C46 H28 Co4 N6 O15
Mr	1140.47	1140.46
Dx,g cm-3	1.754	1.754
Z	4	4
Mu (mm-1)	1.593	1.593
F000	2296.0	2296.0
F000’	2302.54	
h,k,lmax	35,17,13	35,17,13
Nref	8498	8189
Tmin,Tmax	0.892,0.938	0.832,0.939
Tmin’	0.826	

```
Correction method= MULTI-SCAN

Data completeness= 0.964          Theta(max)= 26.000

R(reflections)= 0.0805( 7293)     wR2(reflections)= 0.1767( 8189)

S = 1.132                 Npar= 622
```

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 C

```
DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      2.406
           Test value =      2.025
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
```

The relevant atom site should be identified.

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.964
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.41 eA-3
PLAT213_ALERT_2_C Atom N4 has ADP max/min Ratio ..... 3.2 prola
PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio ..... 3.4 prola
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.4 prola
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio ..... 3.3 prola
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.5 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0103 Ang

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Alert level G

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 78.88
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 -- O1 .. 6.0 su
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.15 Ratio
PLAT793_ALERT_4_G The Model has Chirality at C28 (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C29 (Verify) .... S

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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 18/07/2011; check.def file version of 04/07/2011

Datablock CompoundI - ellipsoid plot