checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kla0195

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kla0195

```
Bond precision:  C-C = 0.0063 A          Wavelength=1.54178

Cell:            a=30.2283(4)     b=30.2283(4)     c=14.3753(3)
                 alpha=90         beta=90          gamma=90
Temperature:     200 K
```

	Calculated	Reported
Volume	13135.4(4)	13135.4(4)
Space group	I 41/a	I4(1)/a
Hall group	-I 4ad	?
Moiety formula	C33 H31 B N9 O3 Tl	?
Sum formula	C33 H31 B N9 O3 Tl	C33 H31 B N9 O3 Tl
Mr	816.86	816.85
Dx,g cm-3	1.652	1.652
Z	16	16
Mu (mm-1)	9.854	9.854
F000	6432.0	6432.0
F000’	6381.23	
h,k,lmax	36,36,17	36,35,16
Nref	6239	6060
Tmin,Tmax	0.459,0.674	0.285,0.677
Tmin’	0.178	

```
Correction method= NUMERICAL

Data completeness= 0.971          Theta(max)= 70.130

R(reflections)= 0.0258( 5178)     wR2(reflections)= 0.0694( 6060)

S = 1.024                 Npar= 430
```

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 B

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C8

Author Response: Atom C8 is part of one of the phenyl rings. Atom identity consistent with synthesis and spectroscopy.

Alert level C

```
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        3.7 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C10
PLAT331_ALERT_2_C Small Average Phenyl   C-C Dist. C5     -C10          1.37 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N9     -   H9A    ...          ?
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         83
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............         3
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      20.03
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         62
```

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 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 05/11/2012; check.def file version of 05/11/2012

Datablock kla0195 - ellipsoid plot