checkCIF/PLATON report

Structure factors have been supplied for datablock(s) apx539_fulla

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: apx539_fulla

```
Bond precision:  C-C = 0.0127 A          Wavelength=0.71073

Cell:            a=11.199(6)    b=34.737(18)         c=10.931(6)
                 alpha=90       beta=116.801(7)      gamma=90
Temperature:     140 K
```

	Calculated	Reported
Volume	3796(4)	3795(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H60 Ce O2 Si4	?
Sum formula	C30 H60 Ce O2 Si4	C30 H60 Ce O2 Si4
Mr	705.26	705.26
Dx,g cm-3	1.234	1.234
Z	4	4
Mu (mm-1)	1.347	1.348
F000	1480.0	1480.0
F000’	1480.61	
h,k,lmax	13,42,13	13,42,13
Nref	7291	7265
Tmin,Tmax	0.851,0.898	0.874,0.898
Tmin’	0.851	

```
Correction method= # Reported T Limits: Tmin=0.874 Tmax=0.898
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.782

R(reflections)= 0.0696( 3776)     wR2(reflections)= 0.1775( 7265)

S = 0.966                 Npar= 352
```

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.206

Alert level C

PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	4.3 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H	Uiso(max)/Uiso(min) ...	5.4 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference Si1 -- C6 ..		0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C23 -- C24 ..		0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C27 -- C29 ..		0.21 Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Si1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Si4 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.01269 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		6.018 Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600		5 Report
PLAT972_ALERT_2_C	Check Calcd Residual Density 0.87A From	Ce1	-1.92 eA-3
PLAT972_ALERT_2_C	Check Calcd Residual Density 0.93A From	Ce1	-1.70 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Residual Density on	Ce1	1.04 eA-3
PLAT975_ALERT_2_C	Check Calcd Residual Density 1.02A From	O2	0.50 eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		9 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		4 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		2 Report
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =		8 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		31 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...		1 Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		20 Note

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

0 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
8 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
0 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 19/11/2015; check.def file version of 17/11/2015

Datablock apx539_fulla - ellipsoid plot