checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

No syntax errors found. CIF dictionary Interpreting this report

Datablock: x

```
Bond precision:  C-C = 0.0035 A          Wavelength=0.71073

Cell:            a=9.0021(10)     b=14.9816(18)     c=16.5464(19)
                 alpha=90         beta=90           gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	2231.5(4)	2231.5(4)
Space group	P 21 21 21	P 212121
Hall group	P 2ac 2ab	?
Moiety formula	C21 H32 N2 O3 S	C21 H32 N2 O3 S
Sum formula	C21 H32 N2 O3 S	C21 H32 N2 O3 S
Mr	392.56	392.55
Dx,g cm-3	1.168	1.168
Z	4	4
Mu (mm-1)	0.167	0.167
F000	848.0	848.0
F000’	848.83	
h,k,lmax	10,17,19	10,17,19
Nref	2265[3964]	3961
Tmin,Tmax	0.940,0.953	0.805,0.953
Tmin’	0.940	

```
Correction method= MULTI-SCAN

Data completeness= 1.75/1.00      Theta(max)= 25.080

R(reflections)= 0.0367( 3270)     wR2(reflections)= 0.0977( 3961)

S = 1.021                 Npar= 274
```

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for N1 -- C1 .. 7.5 su

Alert level C

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    O2     --  C1      ..        5.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C16    --  C17     ..        5.3 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         O2
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C8
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C18
```

Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           25.08
          From the CIF: _reflns_number_total               3961
          Count of symmetry unique reflns         2265
          Completeness (_total/calc)           174.88%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      1696
          Fraction of Friedel pairs measured     0.749
          Are heavy atom types Z>Si present        yes
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in CIF ...          ?
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for        C3A
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for        C3B
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................         22 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3
PLAT791_ALERT_4_G Note: The Model has Chirality at C12    (Verify)          R
PLAT791_ALERT_4_G Note: The Model has Chirality at C14    (Verify)          S
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..       0.07
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still          54 Perc.
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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
  11 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   5 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 22/10/2012; check.def file version of 16/10/2012

Datablock x - ellipsoid plot