checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: shelx

```
Bond precision:   C-C = 0.0126 A          Wavelength=0.71073

Cell:               a=6.1196(19)      b=15.078(4)      c=23.215(7)
                    alpha=90          beta=90          gamma=90
Temperature:        273 K
```

	Calculated	Reported
Volume	2142.1(11)	2142.0(11)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C22 H33 N O4 S	C22 H33 N O4 S
Sum formula	C22 H33 N O4 S	C22 H33 N O4 S
Mr	407.55	407.55
Dx,g cm-3	1.264	1.264
Z	4	4
Mu (mm-1)	0.178	0.178
F000	880.0	880.0
F000'	880.87	
h,k,lmax	7,18,28	7,18,28
Nref	4217[2444]	4178
Tmin,Tmax	0.979,0.995	0.947,0.986
Tmin'	0.953	

```
Correction method= # Reported T Limits: Tmin=0.947 Tmax=0.986
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.99        Theta(max)= 25.994

R(reflections)= 0.1055( 3772)                    wR2(reflections)=
                                                 0.2439( 4178)
S = 1.221                  Npar= 252
```

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01257 Ang.

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio ..... 3.2 oblate
PLAT213_ALERT_2_C Atom C14 has ADP max/min Ratio ..... 3.2 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.12 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 273 Check
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C5 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C10 (Sohnke SpGr) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 37 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree

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

3 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
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* or *IUCrData*, 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 28/11/2022; check.def file version of 28/11/2022

Datablock shelx - ellipsoid plot