checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

```
Bond precision:   C-C = 0.0042 A          Wavelength=0.71073

Cell:               a=9.834(9)     b=12.609(10)       c=16.946(16)
                    alpha=90       beta=90.94(3)      gamma=90
Temperature:        100 K
```

	Calculated	Reported
Volume	2101(3)	2101(3)
Space group	P c	P 1 c 1
Hall group	P -2yc	P -2yc
Moiety formula	2(C14 H22 N3 O2 S), 2(C4 H5 O4), C2 H6 O	2(C14 H22 N3 O2 S), 2(C4 H5 O4), C2 H6 O
Sum formula	C38 H60 N6 O13 S2	C38 H60 N6 O13 S2
Mr	873.04	873.04
Dx,g cm-3	1.380	1.380
Z	2	2
Mu (mm-1)	0.198	0.198
F000	932.0	932.0
F000'	932.95	
h,k,lmax		14,18,24
Nref		10388
Tmin,Tmax	0.926,0.959	0.460,0.746
Tmin'	0.926	

```
Correction method= # Reported T Limits: Tmin=0.460 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 30.893

R(reflections)= 0.0467( 9088)                  wR2(reflections)=
                                               0.1188( 10388)
S = 1.025                  Npar= 576
```

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

```
PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro ....     Please Do !
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Author Response: Flack for a twinned crystal coincides with BASF. Hooft is equal to -0.05(5).

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PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00424 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         69 Report
                  9  0  0,  10  0  0,  11  0  0,   9  1  0,  10  1  0,  11  1  0,
                 10  2  0,  11  2  0,  10  3  0,  11  3  0,  11  4  0, -11  1  1,
                  7  1  1,   8  1  1,   9  1  1,  10  1  1,  11  1  1, -11  2  1,
                  8  2  1,   9  2  1,  10  2  1,  11  2  1, -11  3  1,  10  3  1,
                 11  3  1, -11  0  2,   7  0  2,   8  0  2,   9  0  2,  10  0  2,
                 11  0  2,   7  1  2,   8  1  2,   9  1  2,  10  1  2,  11  1  2,
                  9  2  2,  10  2  2,  11  2  2,  11  3  2,  -1  9  2,  -1 10  2,
                  7  1  3,   8  1  3,   9  1  3,  10  1  3,  11  1  3,   9  2  3,
                 10  2  3,  11  2  3,   7  0  4,   8  0  4,   9  0  4,  10  0  4,
                 11  0  4,   8  1  4,   9  1  4,  10  1  4,  11  1  4,   9  2  4,
                 10  2  4,  -3 10  4,   9  1  5,  10  1  5,   8  0  6,   9  0  6,
                 10  0  6,   6  0 12,   8  0 12,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         18 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         21 Note
                  H1AA    H2AA    H1AB    H1AC    H1AD    H2AB    H2AC    H2BA
                  H2BB    H3BA    H3BB    H2CA    H2CB    C3BC    H3BC    H3BD
                  H1SA    H1SB    H2SA    H2SB    H2SC
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         11 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                  0  1  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        149 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         60 %
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         11 Info
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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
   4 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   3 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* 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 14/11/2023; check.def file version of 14/09/2023

Datablock a - ellipsoid plot