checkCIF/PLATON report

Structure factors have been supplied for datablock(s) RA18.9

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: RA18.9

Bond precision: C-C = 0.0030 A   Wavelength=0.71073

Cell: a=11.6565(7)   b=23.8750(14)   c=7.0514(4)
                   alpha=90   beta=90   gamma=90
Temperature: 135 K

	Calculated	Reported
Volume	1962.4(2)	1962.4(2)
Space group	P n n a	P n n a
Hall group	-P 2a 2bc	-P 2a 2bc
Moiety formula	C6 H14 N2 O2, O4 S	?
Sum formula	C6 H14 N2 O6 S	C6 H14 N2 O6 S
Mr	242.25	242.25
Dx,g cm-3	1.640	1.640
Z	8	8
Mu (mm-1)	0.344	0.344
F000	1024.0	1024.0
F000'	1025.60	
h,k,lmax	14,28,8	14,28,8
Nref	1800	1796
Tmin,Tmax	0.898,0.950	0.986,1.000
Tmin'	0.791	

Correction method= # Reported T Limits: Tmin=0.986 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998   Theta(max)= 25.350

R(reflections)= 0.0314(1564)   wR2(reflections)= 0.0824(1796)

S = 1.060   Npar= 142

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

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.364 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=     0.600         2 Report
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..     0.68 mm
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4S       ..C13       .     2.99 Ang.
                                  1/2+x,y,1-z  =     6_656 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.0 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   0 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
   5 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 12/09/2022; check.def file version of 09/08/2022

Datablock RA18.9 - ellipsoid plot