checkCIF/PLATON report

Structure factors have been supplied for datablock(s) burm002

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: burm002

Bond precision: C-C = 0.0016 A   Wavelength=0.71073

Cell: a=11.4315(3)   b=6.6765(2)   c=11.5969(3)
                   alpha=90   beta=107.8509(5)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	842.49(4)	842.49(4)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	C18 H22 N4 O3 S	C18 H22 N4 O3 S
Sum formula	C18 H22 N4 O3 S	C18 H22 N4 O3 S
Mr	374.46	374.45
Dx,g cm-3	1.476	1.476
Z	2	2
Mu (mm-1)	0.220	0.220
F000	396.0	396.0
F000'	396.40	
h,k,lmax	15,8,15	15,8,15
Nref	2269	2268
Tmin,Tmax	0.937,0.952	0.870,0.958
Tmin'	0.927	

Correction method= # Reported T Limits: Tmin=0.870 Tmax=0.958
AbsCorr = NUMERICAL

Data completeness= 1.000   Theta(max)= 28.304

R(reflections)= 0.0284(2195)   wR2(reflections)= 0.0800(2268)

S = 1.045   Npar= 198

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**
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C5   - C6   .   1.53 Ang.

● **Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   21 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   2 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0050 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0050 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C20 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C40 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   20 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   42 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   10 Info

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **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

   1 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
   4 ALERT type 3 Indicator that the structure quality may be low
   4 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 28/11/2022; check.def file version of 28/11/2022

Datablock burm002 - ellipsoid plot