checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_is_3_75_0m

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: mo_is_3_75_0m

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

Cell:             a=11.0164(3)     b=7.4894(2)         c=21.0540(7)
                  alpha=90         beta=97.435(1)      gamma=90
Temperature:      101 K

                 Calculated                Reported
Volume           1722.48(9)                1722.48(9)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C19 H19 O2 P S2           C19 H19 O2 P S2
Sum formula      C19 H19 O2 P S2           C19 H19 O2 P S2
Mr               374.43                    374.43
Dx,g cm-3        1.444                     1.444
Z                4                         4
Mu (mm-1)        0.411                     0.411
F000             784.0                     784.0
F000'            785.67
h,k,lmax         16,11,32                  16,11,32
Nref             6610                      6600
Tmin,Tmax        0.988,0.992               0.721,0.747
Tmin'            0.848

Correction method= # Reported T Limits: Tmin=0.721 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 33.204

R(reflections)= 0.0378( 5909)                wR2(reflections)=
                                             0.1129( 6600)
S = 1.055                  Npar= 218
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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

```
PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density ....       4.97 Report
PLAT975_ALERT_2_B Check Calcd Resid. Dens.  1.00Ang From O004    .       1.52 eA-3
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Alert level C

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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
          The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       1.59 eA-3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
               2  0  0,   2  1  1,  -3  1  4,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
               1  1  0,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From O004            1.52 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From O005    .       0.46 eA-3
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Alert level G

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         43 Note
             S001    P002    S003    O004    O005    C006    H006    C007
             C008    H008    C009    C00A    H00A    C00B    H00B    H00C
             C00C    H00D    C00D    C00E    H00E    C00F    H00F    C00G
             C00H    H00H    C00I    H00I    C00J    H00J    C00K    H00G
             H00K    H00L    C00L    H00M    H00N    C00M    H00O    C00N
             H00P    C00O    H00Q
PLAT793_ALERT_4_G Model has Chirality at C008        (Centro SpGr)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C00C        (Centro SpGr)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C00I        (Centro SpGr)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C00J        (Centro SpGr)          R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               1  0  0,  -1  0  2,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
              -3  1  4,   0  0  2,   1  0  0,   2  1  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.004 Note
             Predicted wR2: Based on SigI**2  2.26 or SHELX Weight 10.70
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   7 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   6 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 02/02/2025; check.def file version of 02/02/2025

Datablock mo_is_3_75_0m - ellipsoid plot