checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_cammiade_ac82_0m_5

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_cammiade_ac82_0m_5

```
Bond precision:   C-C = 0.0065 A          Wavelength=0.71073

Cell:           a=8.833(3)        b=9.691(3)        c=18.674(6)
                alpha=98.274(7)   beta=93.305(10)   gamma=107.308(9)
Temperature:    100 K

                 Calculated                Reported
Volume           1501.7(8)                 1501.6(8)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C26 H30 Mg2 N2 O14        ?
Sum formula      C26 H30 Mg2 N2 O14        C26 H30 Mg2 N2 O14
Mr               643.14                    643.14
Dx,g cm-3        1.422                     1.422
Z                2                         2
Mu (mm-1)        0.152                     0.152
F000             672.0                     672.0
F000'            672.55
h,k,lmax         10,11,22                  10,11,22
Nref             5527                      5584
Tmin,Tmax        0.983,0.989               0.667,0.743
Tmin'            0.983

Correction method= # Reported T Limits: Tmin=0.667 Tmax=0.743
AbsCorr = MULTI-SCAN

Data completeness= 1.010           Theta(max)= 25.392

R(reflections)= 0.0744( 3996)                wR2(reflections)=
                                             0.1659( 5584)
S = 1.032                 Npar= 407
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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

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PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       1.36 eA-3
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        7.0 Ratio
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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.
PLAT213_ALERT_2_C Atom C19            has ADP max/min Ratio .....        3.2 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        7.3 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O12 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0065 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H25B     ..H25B     .       2.10 Ang.
                                          1-x,2-y,1-z  =      2_676 Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         66 Ang**3
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.519 Check
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           1 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
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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
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 28/11/2022; check.def file version of 28/11/2022

Datablock mo_cammiade_ac82_0m_5 - ellipsoid plot