checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_IALVB118_0m_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: mo_IALVB118_0m_a

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Bond precision:   C-C = 0.0070 A          Wavelength=0.71073

Cell:             a=11.1935(4)     b=24.2208(7)         c=15.5561(5)
                  alpha=90         beta=103.718(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           4097.2(2)                 4097.2(2)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C42 H30 F9 N2 O6 Tb       C42 H30 F9 N2 O6 Tb
Sum formula      C42 H30 F9 N2 O6 Tb       C42 H30 F9 N2 O6 Tb
Mr               988.61                    988.60
Dx,g cm-3        1.603                     1.603
Z                4                         4
Mu (mm-1)        1.816                     1.816
F000             1960.0                    1960.0
F000'            1960.52
h,k,lmax         12,27,17                  12,27,17
Nref             6332                      6318
Tmin,Tmax        0.715,0.817               0.650,0.745
Tmin'            0.701

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 23.857

R(reflections)= 0.0323( 5875)                wR2(reflections)=
                                             0.0736( 6318)
S = 1.144                  Npar= 547
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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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5691

Author Response: The value of sine(theta_max)/wavelength is 0.5824, because crystals were poorly diffracting at high angles. Other attempts of crystallization were done, but no single crystals of better quality were obtaine

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Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio

Author Response: Due to the quality of the crystal there was litle dinamic disordered O crystallization were done, but no single crystals of better quality were obtaine

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C41 Check

Author Response: Due to the quality of the crystal there was litle dinamic disordered O crystallization were done, but no single crystals of better quality were obtaine

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.383 Check

Author Response: Due to the quality of the crystal we have not taken in account some re angles which intensity values were negative. Other attempts of crystallization were done, but no single crystals of better qu

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.569 12 Report

Author Response: These reflections were probably affected by unexpected deviations in their intensities for symmetry equivalent measurements and omitted during initial data reduction. Other attempts of crystallization were done, but no single crystals of better qu

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.78 Why ?

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PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F4A      --C23      .        7.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F4B      --C23      .        6.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F5B      --C23      .       13.0 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C33 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         5% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Tb1       (III)     .      3.39 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        21 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         85% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
3 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 13/07/2021; check.def file version of 13/07/2021

Datablock mo_IALVB118_0m_a - ellipsoid plot