checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a_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: a_a

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Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:           a=6.3740(8)    b=19.523(2)         c=11.3239(14)
                alpha=90       beta=104.066(3)     gamma=90
Temperature:    120 K

                Calculated                Reported
Volume          1366.9(3)                 1366.9(3)
Space group     P 21                      P 21
Hall group      P 2yb                     P 2yb
Moiety formula  C18 H22 O                 C18 H22 O
Sum formula     C18 H22 O                 C18 H22 O
Mr              254.36                    254.35
Dx,g cm-3       1.236                     1.236
Z               4                         4
Mu (mm-1)       0.074                     0.074
F000            552.0                     552.0
F000'           552.22
h,k,lmax        8,26,15                   8,26,15
Nref            7276[ 3740]               7273
Tmin,Tmax       0.991,0.994               0.817,0.960
Tmin'           0.969

Correction method= # Reported T Limits: Tmin=0.817 Tmax=0.960
AbsCorr = MULTI-SCAN

Data completeness= 1.94/1.00      Theta(max)= 28.998

R(reflections)= 0.0605( 5073)     wR2(reflections)= 0.1368( 7273)

S = 0.998                 Npar= 351
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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

PLAT035_ALERT_1_B _chemical_absolute_configuration Info Not Given Please Do !

Author Response: The crystal is pseudoracemate - two indepdent molecules are enantiomers.

PLAT420_ALERT_2_B D-H Without Acceptor O1A --H1OA . Please Check

Author Response: Due to the lack of hydrogen atoms acceptor in the molecule the OH group of one of the indepdent molecules don't participate in the formation of H-bond

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Alert level C

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 2.200
From the CIF: _refine_ls_abs_structure_Flack_su 1.000
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00505 Ang.
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 2.20 Check

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Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT115_ALERT_5_G ADDSYM Detects Noncrystallographic Inversion ... 94% Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 14 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.68 Check
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 4 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 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

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 07/08/2019; check.def file version of 30/07/2019

Datablock a_a - ellipsoid plot