checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 220128a

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: 220128a

```
Bond precision:   C-C = 0.0109 A          Wavelength=0.71073

Cell:             a=5.8638(6)     b=22.871(2)         c=14.5987(14)
                  alpha=90        beta=97.316(3)      gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	1941.9(3)	1941.9(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H17 O3 P	C22 H17 O3 P
Sum formula	C22 H17 O3 P	C22 H17 O3 P
Mr	360.33	360.32
Dx,g cm-3	1.232	1.232
Z	4	4
Mu (mm-1)	0.159	0.159
F000	752.0	752.0
F000'	752.74	
h,k,lmax	6,27,17	6,27,17
Nref	3412	3380
Tmin,Tmax	0.987,0.995	0.883,0.995
Tmin'	0.881	

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Correction method= # Reported T Limits: Tmin=0.883 Tmax=0.995
AbsCorr = MULTI-SCAN

Data completeness= 0.991           Theta(max)= 25.019

R(reflections)= 0.0936( 1080)                    wR2(reflections)=
                                                 0.1926( 3380)
S = 0.864                  Npar= 236
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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

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 32% Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01091 Ang.

Alert level C

PLAT234_ALERT_4_C Large Hirshfeld Difference C4 --C9 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C19 --C20 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20 --C21 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 366.241 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 11.238 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 38.526 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 14.775 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 18.382 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.945 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 9.924 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.064 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.267 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.015 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 31 Report

Alert level G

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.80 mm
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C4 -C9 . 1.42 Ang.
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 . 103.8 Degree
PLAT793_ALERT_4_G Model has Chirality at P1 (Centro SPGR) S Verify
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT930_ALERT_2_G FCF-based Twin Law (0 2-1) Est.d BASF 0.63 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (0 2-1) Est.d BASF 0.63 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 18 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.0 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 15 ALERT type 3 Indicator that the structure quality may be low
  6 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 12/09/2022; check.def file version of 09/08/2022

Datablock 220128a - ellipsoid plot