checkCIF/PLATON report

Structure factors have been supplied for datablock(s) md3a

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: md3a

Bond precision: C-C = 0.0043 A   Wavelength=0.71073

Cell: a=10.3939(4)   b=14.7587(5)   c=8.0940(5)
                 alpha=90   beta=97.683(4)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1230.48(10)	1230.48(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H8 Ag F2 N2 O2 P	C12 H8 Ag F2 N2 O2 P
Sum formula	C12 H8 Ag F2 N2 O2 P	C12 H8 Ag F2 N2 O2 P
Mr	389.04	389.04
Dx,g cm-3	2.100	2.100
Z	4	4
Mu (mm-1)	1.794	1.794
F000	760.0	760.0
F000'	757.17	
h,k,lmax	12,17,9	12,17,9
Nref	2198	2192
Tmin,Tmax	0.727,0.931	0.553,0.919
Tmin'	0.621	

Correction method= # Reported T Limits: Tmin=0.553 Tmax=0.919
AbsCorr = INTEGRATION

Data completeness= 0.997   Theta(max)= 25.118

R(reflections)= 0.0269(1899)   wR2(reflections)= 0.0711(2192)

S = 1.047   Npar= 181

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 C

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      O1 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      P1 Check
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        2 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)      293 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 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 18/02/2019; check.def file version of 18/02/2019

NOMOVE FORCED

Prob = 50
Temp = 293

61 Y

PLATON-Feb 25 16:00:53 2019 - (70316)

Z -88   md3a   P 1 21/c 1   R = 0.03   RES=   0   170 X