checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bake12

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: bake12

Bond precision: C-C = 0.0061 A   Wavelength=1.34139

Cell: a=9.0038(3)   b=13.9811(5)   c=13.4556(5)
                alpha=90   beta=107.861(2)   gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1612.20(10)	1612.19(10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H11 F3 Mn N3 O2	C18 H11 F3 Mn N3 O2
Sum formula	C18 H11 F3 Mn N3 O2	C18 H11 F3 Mn N3 O2
Mr	413.24	413.24
Dx,g cm-3	1.702	1.703
Z	4	4
Mu (mm-1)	4.890	4.890
F000	832.0	832.0
F000'	834.12	
h,k,lmax	11,17,16	11,17,16
Nref	3183	3133
Tmin,Tmax	0.746,0.864	0.255,0.369
Tmin'	0.584	

Correction method= # Reported T Limits: Tmin=0.255 Tmax=0.369
AbsCorr = MULTI-SCAN

Data completeness= 0.984   Theta(max)= 56.026

R(reflections)= 0.0574(2296)   wR2(reflections)= 0.1475(3133)

S = 1.036   Npar= 245

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

```
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00607 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.967 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mn1        --C16        .      6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mn1        --C17        .      7.5 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C16 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (I)       .   0.96 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600       43 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       2 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 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
   4 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
   1 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.