

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0098 A Wavelength=0.71073

Cell: a=6.9984(5) b=9.9870(9) c=10.8023(8)
 alpha=88.652(3) beta=71.277(2) gamma=75.664(2)

Temperature: 200 K

	Calculated	Reported
Volume	691.50(10)	691.50(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H8 F3 Mn N2 O3	?
Sum formula	C14 H8 F3 Mn N2 O3	C14 H8 F3 Mn N2 O3
Mr	364.16	364.16
Dx,g cm-3	1.749	1.749
Z	2	2
Mu (mm-1)	1.006	1.006
F000	364.0	364.0
F000'	364.89	
h,k,lmax	8,12,13	8,12,13
Nref	2838	8801
Tmin,Tmax	0.798,0.943	0.645,0.745
Tmin'	0.794	

Correction method= # Reported T Limits: Tmin=0.645 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 3.101 Theta(max)= 26.375

R(reflections)= 0.0846(5248) wR2(reflections)= 0.1456(8801)

S = 1.048 Npar= 209

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	0.00978	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2 .. F3 ..	2.59	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	7.953	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	2.065	Check

Alert level G

PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	84	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT341_shelx
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00978 Ang.
RESPONSE: ...
;
_vrf_PLAT480_shelx
;
PROBLEM: Long H...A H-Bond Reported H2 .. F3 .. 2.59 Ang.
RESPONSE: ...
;
_vrf_PLAT906_shelx
;
PROBLEM: Large K value in the Analysis of Variance ..... 7.953 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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.

