

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_188

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: exp\_188

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Bond precision:    C-C = 0.0051 Å                      Wavelength=0.71073

Cell:                      a=6.0290 (7)                      b=8.1542 (10)                      c=13.4778 (17)  
                            alpha=79.481 (10)                      beta=86.443 (10)                      gamma=75.029 (10)  
Temperature:    295 K

	Calculated	Reported
Volume	629.27 (14)	629.27 (14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H12 F3 N O3	C13 H12 F3 N O3
Sum formula	C13 H12 F3 N O3	C13 H12 F3 N O3
Mr	287.24	287.24
Dx, g cm <sup>-3</sup>	1.516	1.516
Z	2	2
Mu (mm <sup>-1</sup> )	0.136	0.136
F000	296.0	296.0
F000'	296.22	
h, k, lmax	8, 11, 19	8, 11, 18
Nref	3993	3339
Tmin, Tmax	0.954, 0.977	0.810, 1.000
Tmin'	0.946	

Correction method= # Reported T Limits: Tmin=0.810 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.836                      Theta(max)= 30.915

R(reflections)= 0.0702 ( 1620)	wR2(reflections)=
S = 1.015	0.2335 ( 3339)
Npar= 186	

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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.

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#### Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49% Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C13 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00508 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.412 Report
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	38 Report

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#### Alert level G

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....	Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.01 Degree
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C1 Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4	104.4 Degree
PLAT793_ALERT_4_G	Model has Chirality at C5 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	R Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	595 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	5 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
9 **ALERT level G** = General information/check it is not something unexpected

- 2 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  
5 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
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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.

