

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk1776

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: bmk1776

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Bond precision:      C-C = 0.0033 Å      Wavelength=0.71073

Cell:                      a=11.4945(5)                      b=14.8707(6)                      c=16.2570(6)  
                             alpha=96.807(3)                      beta=95.999(4)                      gamma=106.731(4)  
Temperature:              296 K

	Calculated	Reported
Volume	2614.2(2)	2614.20(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H21 F3 N8 S	?
Sum formula	C28 H21 F3 N8 S	C28 H21 F3 N8 S
Mr	558.59	558.59
Dx, g cm <sup>-3</sup>	1.419	1.419
Z	4	4
Mu (mm <sup>-1</sup> )	0.180	0.180
F000	1152.0	1152.0
F000'	1152.99	
h, k, lmax	16, 20, 22	16, 20, 22
Nref	15124	11910
Tmin, Tmax	0.967, 0.988	0.643, 1.000
Tmin'	0.925	

Correction method= # Reported T Limits: Tmin=0.643 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 0.787      Theta(max)= 29.921

R(reflections)= 0.0508( 7393)	wR2(reflections)=
S = 1.012	0.1523( 11910)
Npar= 725	

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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 B

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min).

14 Note

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#### Alert level C

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C53 --C54 . 6.0 s.u.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C55 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C26 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C51 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C54 Check  
PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C1 -C6 . 1.36 Ang.  
PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C23 -C28 . 1.37 Ang.  
PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C29 -C34 . 1.37 Ang.  
PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C41 -C46 . 1.37 Ang.  
PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C51 -C56 . 1.37 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 7.578 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 45 Report

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#### Alert level G

PLAT793\_ALERT\_4\_G Model has Chirality at C12 (Centro SPGR) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C40 (Centro SPGR) S Verify  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 3156 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.1 Low  
PLAT962\_ALERT\_5\_G Number FCF File Reflections with Sigma(I) = 0.0 4 Note  
PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info  
PLAT992\_ALERT\_5\_G Repd & Actual \_reflns\_number\_gt Values Differ by 6 Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

13 **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

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

13 ALERT type 2 Indicator that the structure model may be wrong or deficient

4 ALERT type 3 Indicator that the structure quality may be low

3 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.

