

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 24090400520240904\_auto

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: 24090400520240904\_auto

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Bond precision:      C-C = 0.0033 Å      Wavelength=1.54184

Cell:                      a=9.5689(1)              b=10.7033(1)              c=16.9732(1)  
                                alpha=90              beta=90              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	1738.38(3)	1738.37(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C20 H23 N O2 S	C20 H23 N O2 S
Sum formula	C20 H23 N O2 S	C20 H23 N O2 S
Mr	341.45	341.48
Dx, g cm <sup>-3</sup>	1.305	1.305
Z	4	4
Mu (mm <sup>-1</sup> )	1.740	1.741
F000	728.0	731.5
F000'	731.21	
h,k,lmax	12,13,21	11,13,21
Nref	3672[ 2105]	3495
Tmin,Tmax	0.741,0.706	0.630,1.000
Tmin'	0.672	

Correction method= # Reported T Limits: Tmin=0.630 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.95      Theta(max)= 76.960

R(reflections)= 0.0408( 3473)	wR2(reflections)= 0.1017( 3495)
S = 1.039	Npar= 218

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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

PLAT213\_ALERT\_2\_C Atom C000 has ADP max/min Ratio ..... 3.1 prolat  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.6 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.7 Ratio  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C000 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C00K Check  
PLAT414\_ALERT\_2\_C Short Intra D-H..H-X H005 ..H004 . 1.96 Ang.  
x,y,z = 1\_555 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report  
2 0 0, 1 3 0, 1 1 1, 2 1 1, 1 2 1, 0 2 2,  
1 2 2, 1 0 3, 0 2 3, 1 2 3, 0 0 4, 0 3 4,  
1 0 5,  
PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 8 Note  
2 0 0, 0 1 1, 2 1 1, 1 2 2, 1 0 3, 0 2 3,  
1 2 3, 0 3 4,  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 1.01Ang From N004 . -0.42 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H004 . -0.39 eA-3

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### Alert level G

PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT073\_ALERT\_1\_G H-atoms ref, but \_hydrogen\_treatment Reported as constr Check  
PLAT142\_ALERT\_4\_G s.u. on b - Axis Small or Missing ..... 0.00010 Ang.  
PLAT143\_ALERT\_4\_G s.u. on c - Axis Small or Missing ..... 0.00010 Ang.  
PLAT153\_ALERT\_1\_G The s.u.'s on the Cell Axes are Equal ..(Note) 0.0001 Ang.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 47 Note  
S001 O002 O003 N004 C005 C006 C007 C008  
C009 C00A C00B C00C C00D C00E C00F C00G  
C00H C00I C00J C00K C00L C00M C00N C00O  
H00D H00J H00H H00E H00B H00G H008 H00F  
H005 H006 H00I H00A H00C H00K H00L H00M  
H00N H00O H00P H00Q H00R H00S H004  
PLAT769\_ALERT\_4\_G CIF Embedded Explicitly Supplied Scattering Data Please Note  
PLAT791\_ALERT\_4\_G Model has Chirality at C006 (Sohncke SpGr) R Verify  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
0 1 1,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 48 Note  
PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... Please Check  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 8.573 Note  
Predicted wR2: Based on SigI\*\*2 1.19 or SHELX Weight 9.78  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 7 Info  
PLAT982\_ALERT\_1\_G The C-f'= 0.0192 Deviates from IT-value = 0.0181 Check  
PLAT982\_ALERT\_1\_G The N-f'= 0.0326 Deviates from IT-value = 0.0311 Check  
PLAT982\_ALERT\_1\_G The O-f'= 0.0524 Deviates from IT-value = 0.0492 Check  
PLAT982\_ALERT\_1\_G The S-f'= 0.3354 Deviates from IT-value = 0.3331 Check  
PLAT983\_ALERT\_1\_G The O-f''= 0.0338 Deviates from IT-Value = 0.0322 Check  
PLAT983\_ALERT\_1\_G The S-f''= 0.5514 Deviates from IT-Value = 0.5567 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

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 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  
6 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.

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