

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sad

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: sad

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Bond precision:      C-C = 0.0018 Å      Wavelength=0.71073

Cell:                      a=6.6639(2)                      b=10.5197(4)                      c=16.0485(5)  
                              alpha=108.8447(7)                      beta=92.4433(8)                      gamma=98.1904(8)  
Temperature:      120 K

	Calculated	Reported
Volume	1049.14(6)	1049.14(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 H14 B10 N12, C3 H6 O	C7 H14 B10 N12, C3 H6 O
Sum formula	C10 H20 B10 N12 O	C10 H20 B10 N12 O
Mr	432.48	432.48
Dx, g cm <sup>-3</sup>	1.369	1.369
Z	2	2
Mu (mm <sup>-1</sup> )	0.088	0.088
F000	444.0	444.0
F000'	444.08	
h, k, lmax	9, 14, 22	9, 14, 22
Nref	6138	6138
Tmin, Tmax	0.964, 0.995	0.910, 0.995
Tmin'	0.964	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.995  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 29.999

R(reflections)= 0.0426( 4609)	wR2(reflections)=
S = 1.010	0.1184( 6138)
Npar= 392	

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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 G

PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	7% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2 )	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3 )	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 2 )	5.05 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 3 )	4.95 Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C1 Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C2 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C1 - C2 .	1.65 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1S ..C16 .	2.98 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N7 ..C13 .	3.02 Ang.
		1+x,y,z =	1_655 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		12 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.9 Low
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		5 Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		60.0 Degree
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		3 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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
18 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 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  
5 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.

