

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zufz159

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: zufz159

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

Cell:                      a=9.534(3)              b=18.823(4)              c=23.587(4)  
                                    alpha=90              beta=90                      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	4232.9(18)	4232.9(18)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C23 H32 N2 O2	C23 H32 N2 O2
Sum formula	C23 H32 N2 O2	C23 H32 N2 O2
Mr	368.51	368.50
Dx,g cm-3	1.156	1.156
Z	8	8
Mu (mm-1)	0.073	0.073
F000	1600.0	1600.0
F000'	1600.62	
h,k,lmax	13,26,33	13,26,32
Nref	6174	5963
Tmin,Tmax	0.991,0.997	0.692,1.000
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.692 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.966                      Theta(max)= 29.999

R(reflections)= 0.0472( 3084)              wR2(reflections)= 0.0592( 5963)

S = 1.002                                      Npar= 245

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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**

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N2	--	C1	..	8.2	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C3	--	C4	..	8.6	su
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Th(Min)	...				29	Report

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**Alert level C**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O1	--	C1	..	6.0	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N1	--	C1	..	5.4	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N2	--	C2	..	6.7	su
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H19B	..	O1	..		2.61	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	.....				11.731	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	.....				2.121	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600				6	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	....				5	Note

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					2	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....				1	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	....				0.71	mm
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....				1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				175	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	.....					Please Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
3 **ALERT level B** = A potentially serious problem, consider carefully  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 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*, 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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**PLATON version of 21/06/2015; check.def file version of 21/06/2015**

