

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) psu-459pyron-1

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: psu-459pyron-1

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Bond precision:	C-C = 0.0027 Å	Wavelength=0.71073	
Cell:	a=24.996 (6)	b=5.2350 (8)	c=18.116 (3)
	alpha=90	beta=91.106 (18)	gamma=90
Temperature:	295 K		
	Calculated	Reported	
Volume	2370.1 (8)	2370.1 (8)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C13 H14 N2 O2	C13 H14 N2 O2	
Sum formula	C13 H14 N2 O2	C13 H14 N2 O2	
Mr	230.26	230.26	
Dx, g cm <sup>-3</sup>	1.291	1.291	
Z	8	8	
Mu (mm <sup>-1</sup> )	0.089	0.089	
F000	976.0	976.0	
F000'	976.43		
h, k, lmax		33, 7, 24	
Nref		2930	
Tmin, Tmax	0.974, 0.989	0.730, 1.000	
Tmin'	0.956		

Correction method= # Reported T Limits: Tmin=0.730 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness=      Theta(max)= 29.387

R(reflections)= 0.0561 ( 2122)	wR2(reflections)=
S = 1.029	0.1685 ( 2930)
Npar= 182	

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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**

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C8	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10	Check
PLAT334_ALERT_2_C	Small	<C-C>	Benzene Dist. C7 -C12	1.37	Ang.
PLAT906_ALERT_3_C	Large	K	Value in the Analysis of Variance	4.893	Check

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	5	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	12%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels ..... H2AA H2AB H1AA H1AB	4	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 2 0 0, -2 0 2, 0 0 2, 2 0 2,	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	330	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **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  
7 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

