

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: y

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=7.563 (3) b=11.483 (4) c=13.531 (4)
 alpha=76.835 (5) beta=78.866 (5) gamma=77.227 (5)
Temperature: 296 K

	Calculated	Reported
Volume	1103.2 (7)	1103.2 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H19 N5 O2 [+ solvent]	C23 H19 N5 O2
Sum formula	C23 H19 N5 O2 [+ solvent]	C23 H19 N5 O2
Mr	397.43	397.43
Dx, g cm ⁻³	1.196	1.196
Z	2	2
Mu (mm ⁻¹)	0.080	0.080
F000	416.0	416.0
F000'	416.16	
h, k, lmax	9, 13, 16	9, 13, 16
Nref	4106	4059
Tmin, Tmax	0.984, 0.992	0.636, 0.746
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.636 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.499

R(reflections)= 0.0532 (3134)	wR2(reflections)=
S = 1.026	0.1748 (4059)
Npar= 274	

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.

● **Alert level G**

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	Please Check
PLAT014_ALERT_1_G	No	_shelx_fab_checksum Found in CIF	Please Check
PLAT072_ALERT_2_G	SHELXL	First Parameter in WGHT Unusually Large	0.10 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.005 Degree
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		175 A**3
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1 Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.0 Low

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
8 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

