

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: monika-bd1re3

Bond precision: C-C = 0.0046 A Wavelength=0.71073

Cell: a=20.957(5) b=20.957(5) c=37.034(5)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	16265(8)	16265(6)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C23 H28 O4	C92 H112 O16
Sum formula	C23 H28 O4	C92 H112 O16
Mr	368.45	1473.82
Dx,g cm-3	1.204	1.204
Z	32	8
Mu (mm-1)	0.081	0.081
F000	6336.0	6336.0
F000'	6339.08	
h,k,lmax	25,25,45	25,25,45
Nref	8000	7975
Tmin,Tmax	0.981,0.984	0.686,1.000
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.686 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.000

R(reflections)= 0.0624(3827) wR2(reflections)= 0.1913(7975)

S = 1.000 Npar= 496

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 B

PLAT414_ALERT_2_B	Short Intra D-H..H-X	H3	..	H23A	..	1.86	Ang.
PLAT414_ALERT_2_B	Short Intra D-H..H-X	H23B	..	H212	..	1.84	Ang.

Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections too Low				48	%
PLAT147_ALERT_1_C	su on Symmetry Constrained Cell Angle(s)				Please	Check
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O3B	--	C14B	..	6.5	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C1B	--	C2B	..	7.0	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C15B	--	C16B	..	6.0	su
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for				C15B	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for				C16B	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds				0.0046	Ang.

Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF					Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				4	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ					Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by				4.00	Ratio
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as	.				mixed	Check
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by	...				2	Units
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)				293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)				293	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				4	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL					2014	Note

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

- 7 **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
2 **ALERT type 3** Indicator that the structure quality may be low
2 **ALERT type 4** Improvement, methodology, query or suggestion
2 **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*, 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.

PLATON version of 21/04/2015; check.def file version of 09/03/2015

