

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: rup-re

Bond precision: C-C = 0.0095 A Wavelength=0.71073

Cell: a=12.9504(5) b=23.5121(15) c=28.101(2)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	8556.5(9)	8556.5(9)
Space group	P c a 21	Pca 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C23 H27 N O6	C23 H27 N O6
Sum formula	C23 H27 N O6	C23 H27 N O6
Mr	413.46	413.46
Dx,g cm-3	1.284	1.284
Z	16	16
Mu (mm-1)	0.093	0.093
F000	3520.0	3520.0
F000'	3521.87	
h,k,lmax	15,29,34	15,29,34
Nref	16799[8587]	8558
Tmin,Tmax	0.978,0.982	0.817,1.000
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.817 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.00/0.51 Theta(max)= 26.000

R(reflections)= 0.0691(4881) wR2(reflections)= 0.1825(8558)

S = 1.064 Npar= 1082

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	H43	..	H58	..	1.85	Ang.
PLAT414_ALERT_2_B	Short Intra D-H..H-X	H83	..	H99	..	1.83	Ang.
PLAT414_ALERT_2_B	Short Intra D-H..H-X	H113	..	H129	..	1.82	Ang.
PLAT416_ALERT_2_B	Short Intra D-H..H-D	H4	..	H5	..	1.20	Ang.

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
 From the CIF: `_refine_ls_abs_structure_Flack` -0.700
 From the CIF: `_refine_ls_abs_structure_Flack_su` 1.600

PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C4	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C6	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C110	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C112	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	N1	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C5	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C75	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C111	Check
PLAT334_ALERT_2_C	Small Average Benzene	C-C Dist. C -C118	1.37	Ang.
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.0095	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C23 H27 N O6			

Alert level G

PLAT005_ALERT_5_G	No <code>_iucr_refine_instructions_details</code> in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8 Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	1.600 Report
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed Check
PLAT199_ALERT_1_G	Reported <code>_cell_measurement_temperature</code>	(K) 293 Check
PLAT200_ALERT_1_G	Reported <code>_diffrn_ambient_temperature</code>	(K) 293 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C23 H27 N O6	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3 Note
	C23 H27 N O6	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4 Note
	C23 H27 N O6	
PLAT792_ALERT_1_G	The Model has Chirality at C43 (Polar SPGR)	R Verify
PLAT792_ALERT_1_G	The Model has Chirality at C83 (Polar SPGR)	R Verify
PLAT792_ALERT_1_G	The Model has Chirality at C113 (Polar SPGR)	S Verify
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
4 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
8 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

