

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: 151114b

Bond precision: C-C = 0.0055 A Wavelength=1.54178

Cell: a=9.6170(4) b=13.3217(5) c=15.7153(6)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2013.36(14)	2013.36(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C22 H24 N O5	C22 H24 N O5
Sum formula	C22 H24 N O5	C22 H24 N O5
Mr	382.42	382.42
Dx,g cm-3	1.262	1.262
Z	4	4
Mu (mm-1)	0.732	0.732
F000	812.0	812.0
F000'	814.59	
h,k,lmax	11,15,18	11,15,18
Nref	3551[2035]	2991
Tmin,Tmax	0.755,0.757	0.734,0.768
Tmin'	0.685	

Correction method= # Reported T Limits: Tmin=0.734 Tmax=0.768
AbsCorr = MULTI-SCAN

Data completeness= 1.47/0.84 Theta(max)= 66.393

R(reflections)= 0.0498(2766) wR2(reflections)= 0.1422(2991)

S = 1.057 Npar= 260

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 C

STRVA01_ALERT_4_C Flack parameter is too small
 From the CIF: _refine_ls_abs_structure_Flack -0.270
 From the CIF: _refine_ls_abs_structure_Flack_su 0.180
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.73 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00548 Ang.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
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 3 Note
PLAT791_ALERT_4_G Model has Chirality at C3 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) S Verify
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.2 Low

- 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
7 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 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.

