

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: 2

Bond precision: C-C = 0.0083 A Wavelength=1.54184

Cell: a=5.2286(4) b=10.8928(11) c=24.975(2)
 alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1422.4(2)	1422.4(2)
Space group	P 2 21 21	P22121
Hall group	P 2bc 2	?
Moiety formula	C31 H26 N6, 2(H2 O)	?
Sum formula	C31 H30 N6 O2	C15.50 H15 N3 O
Mr	518.61	259.30
Dx,g cm-3	1.211	1.211
Z	2	4
Mu (mm-1)	0.626	0.626
F000	548.0	548.0
F000'	549.57	
h,k,lmax	6,13,30	6,13,30
Nref	2735[1628]	2130
Tmin,Tmax	0.769,0.928	
Tmin'	0.606	

Correction method= Not given

Data completeness= 1.31/0.78 Theta(max)= 70.440

R(reflections)= 0.0854(1462) wR2(reflections)= 0.2399(2130)

S = 1.009 Npar= Npar = 181

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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full Low 0.873 Note
PLAT031_ALERT_4_A Refined Extinction Parameter within Range 0.438 Sigma

🟡 Alert level B

PLAT057_ALERT_3_B Correction for Absorption Required RT(exp) ... 1.21
PLAT230_ALERT_2_B Hirshfeld Test Diff for C7 -- C16_a .. 10.0 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for C16 -- C7_a .. 10.0 su
PLAT420_ALERT_2_B D-H Without Acceptor O3 - H3B ... Please Check

🟢 Alert level C

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 1.100
From the CIF: _refine_ls_abs_structure_Flack_su 1.300
PLAT230_ALERT_2_C Hirshfeld Test Diff for C6 -- C11 .. 5.2 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C15 .. 0.16 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0083 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 94 Ang3
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C31 H26 N6

🟠 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 2 Why ?
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.300 Why ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by 0.50 Ratio
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.80 mm
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.15 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed
PLAT128_ALERT_4_G Alternate Setting for Input Space-Group P22121 P21212 Note
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C2 -C7 0.24 Ang.
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
H2 O

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
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 05/02/2014; check.def file version of 05/02/2014

