

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 191126_bo5e_0m

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: 191126_bo5e_0m

Bond precision: C-C = 0.0041 Å Wavelength=0.71073

Cell: a=14.345(6) b=15.450(6) c=20.591(9)
 alpha=90 beta=99.88(2) gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	4496(3)	4496(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C54 H48 B2 O2, C H2 Cl2	C54 H48 B2 O2, C H2 Cl2
Sum formula	C55 H50 B2 Cl2 O2	C55 H50 B2 Cl2 O2
Mr	835.47	835.47
Dx, g cm-3	1.234	1.234
Z	4	4
Mu (mm-1)	0.187	0.187
F000	1760.0	1760.0
F000'	1761.81	
h, k, lmax	17, 19, 25	17, 19, 25
Nref	9240	9215
Tmin, Tmax	0.950, 0.965	0.690, 0.745
Tmin'	0.930	

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.405

R(reflections)= 0.0735(6606) wR2(reflections)= 0.2315(9215)

S = 1.024 Npar= 588

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

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl1	0.113	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl1A	0.175	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0041	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.758	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		6	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	11	Report

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		6	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.12	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2		3.70	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3		1.31	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		99	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	7	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		8	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		1	Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected
- 0 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
6 ALERT type 3 Indicator that the structure quality may be low
8 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.

