

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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: 3

Bond precision: C-C = 0.0053 A

Wavelength=0.71073

Cell: a=10.3871(8) b=10.5079(7) c=11.1570(9)
 alpha=81.641(6) beta=81.407(7) gamma=83.885(6)
Temperature: 100 K

	Calculated	Reported
Volume	1186.80(16)	1186.80(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H48 Br5 K2 O12 Sb, 2(C3 H7 N O)	Br5 Sb, 2(K), 2(C12 H24 O6), 2(C3 H7 N O)
Sum formula	C30 H62 Br5 K2 N2 O14 Sb	C30 H62 Br5 K2 N2 O14 Sb
Mr	1274.26	1274.31
Dx,g cm-3	1.783	1.783
Z	1	1
Mu (mm-1)	5.022	5.022
F000	632.0	632.0
F000'	630.70	
h,k,lmax	15,15,16	15,15,16
Nref	8666	7098
Tmin,Tmax	0.061,0.605	0.266,1.000
Tmin'	0.014	

Correction method= # Reported T Limits: Tmin=0.266 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.819

Theta(max)= 32.634

R(reflections)= 0.0403(5939)

wR2(reflections)= 0.0933(7098)

S = 1.104

Npar= 253

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

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.948 Why?

Alert level C

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C00R Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N00C Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.292 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 221 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H00Y -0.64 eA-3

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.80 mm
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb01 --Br02 . 9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb01 --Br03 . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb01 --Br00 . 36.7 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 2% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C00Q Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C00S Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 58 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1346 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
7 ALERT type 4 Improvement, methodology, query or suggestion
0 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* 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.

PLATON version of 16/04/2020; check.def file version of 09/03/2020

