

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision: C-C = 0.0053 A

Wavelength=0.71073

Cell: a=10.5860(4) b=10.6601(6) c=11.3458(5)
 alpha=80.574(4) beta=80.343(3) gamma=82.145(4)
Temperature: 250 K

	Calculated	Reported
Volume	1237.29(10)	1237.29(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H48 Br5 O12 Rb2 Sb, 2(C3 H7 N O)	Br5 Sb, 2(Rb), 2(C12 H24 O6), 2.001(C3 H7 N O)
Sum formula	C30 H62 Br5 N2 O14 Rb2 Sb	C30 H62 Br5 N2 O14 Rb2 Sb
Mr	1367.02	1367.05
Dx,g cm-3	1.835	1.835
Z	1	1
Mu (mm-1)	6.603	6.603
F000	668.0	668.0
F000'	664.52	
h,k,lmax	14,14,15	14,14,15
Nref	6775	5954
Tmin,Tmax		0.940,0.940
Tmin'		

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.940
AbsCorr = SPHERE

Data completeness= 0.879

Theta(max)= 29.295

R(reflections)= 0.0278(5106)

wR2(reflections)= 0.0690(5954)

S = 1.027

Npar= 231

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

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 5 Check
O7B N1B C13B C14B C15B

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br1 . 7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br2 . 23.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br3 . 29.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Br1 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 2% Note
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 6.06 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 1.96 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 4) 3.98 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C14B Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C15B Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H6B ..H15H . 2.14 Ang.
1-x,1-y,2-z = 2_667 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 36 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 821 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
22 **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
4 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
1 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 22/04/2020; check.def file version of 09/03/2020

