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 = 0.0048 A Wavelength=0.71073

Cell: a=10.3975(5) b=10.4680(6) c=11.1155(6)
alpha=81.237(5) beta=80.582(4) gamma=82.112(4)
Temperature: 230 K

	Calculated	Reported
Volume	1171.73(11)	1171.73(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24.67 H49.55 Cl5 N0.22 O12.22 Rb2 Sb, 1.778(C3 H7 N O)	Cl5 Sb, 2(Rb), 2(C12 H24 O6), 2(C3 H7 N O)
Sum formula	C30 H62 Cl5 N2 O14 Rb2 Sb	C30 H62 Cl5 N2 O14 Rb2 Sb
Mr	1144.77	1144.75
Dx,g cm-3	1.622	1.622
Z	1	1
Mu (mm-1)	2.995	2.995
F000	578.0	578.0
F000’	576.51	
h,k,lmax	15,15,16	15,15,16
Nref	8642	7718
Tmin,Tmax	0.070,0.133	0.135,0.166
Tmin’	0.036	

Correction method= # Reported T Limits: Tmin=0.135 Tmax=0.166
AbsCorr = MULTI-SCAN

Data completeness= 0.893 Theta(max)= 32.753

R(reflections)= 0.0417(5789) wR2(reflections)= 0.0980(7718)

S = 1.025 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 B

CRYSS02_ALERT_3_B The value of _exptl_crystal_size_min is > 0.6
Minimum crystal size given = 0.673
CRYSS02_ALERT_3_B The value of _exptl_crystal_size_mid is > 0.8
Mid crystal size given = 0.985

Alert level C

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 5 Check
O7 N1 C13 C14 C15
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.383 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H14E -0.31 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 1.00 mm
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Cl1 . 12.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Cl2 . 15.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Cl3 . 23.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 5% 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
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C14 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C15 Check
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set Please Do !
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
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= 0.600 922 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
9 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* 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

Datablock 1 - ellipsoid plot