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 = 0.0150 A Wavelength=0.71073

Cell: a=14.0505(5) b=14.0505(5) c=21.0782(8)
alpha=90 beta=90 gamma=120
Temperature: 138 K

	Calculated	Reported
Volume	3603.7(3)	3603.7(3)
Space group	R 3	R 3
Hall group	R 3	R 3
Moiety formula	C27 H55 Ba Br6 N O13 Rb Sb, 0.5(C3 H7 N O)	C15 H31 Ba1 N1 O7, Br6 Sb1, C12 H24 O6 Rb1, 0.5(C3 H7 N O)
Sum formula	C28.50 H58.50 Ba Br6 N1.50 O13.50 Rb Sb	C28.50 H58.50 Ba Br6 N1.50 O13.50 Rb Sb
Mr	1462.23	1462.28
Dx,g cm-3	2.021	2.021
Z	3	3
Mu (mm-1)	7.426	7.426
F000	2106.0	2106.0
F000’	2096.63	
h,k,lmax	21,21,32	21,21,31
Nref	5928[2964]	5316
Tmin,Tmax		0.912,0.912
Tmin’		

Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.912
AbsCorr = SPHERE

Data completeness= 1.79/0.90 Theta(max)= 32.708

R(reflections)= 0.0257(4697) wR2(reflections)= 0.0618(5316)

S = 1.063 Npar= 155

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

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.390
From the CIF: _refine_ls_abs_structure_Flack_su 0.010
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ba1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rb1 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.015 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.390 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.99 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br1 . 19.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br2 . 23.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O5 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10C Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11A Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11C Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14C Constrained at 0.1667 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 9% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H6A ..H10B . 2.01 Ang.
1/3-x+y,2/3-x,-1/3+z = 9_554 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H2A ..H14B . 1.97 Ang.
4/3-x+y,5/3-x,-1/3+z = 9_664 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H2B ..H13B . 1.82 Ang.
4/3-y,2/3+x-y,-1/3+z = 8_654 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H5A ..H13C . 2.05 Ang.

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                                      4/3-y,2/3+x-y,-1/3+z  =      8_654 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H5B      ..H13C     .       1.95 Ang.
                                      4/3-y,2/3+x-y,-1/3+z  =      8_654 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         24 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1       (III)     .       2.76 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        174 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  43 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  32 ALERT type 4 Improvement, methodology, query or suggestion
   2 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.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock 1 - ellipsoid plot