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 = 0.0100 A Wavelength=0.71073

Cell: a=8.9339(2) b=13.8500(4) c=24.0142(7)
alpha=80.825(2) beta=86.605(2) gamma=89.767(2)
Temperature: 200 K

	Calculated	Reported
Volume	2928.18(14)	2928.18(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C30 H62 Ba2 Br6 N2 O14 Sb), 2(C1.50 H3.50 Br4 N0.50 O0.50 Sb)	C30 H62 Ba2 Br6 N2 O14 Sb, C1.5 H3.5 Br4 N0.5 O0.5 Sb
Sum formula	C63 H131 Ba4 Br20 N5 O29 Sb4	C31.50 H65.50 Ba2 Br10 N2.50 O14.50 Sb2
Mr	4057.09	2028.64
Dx,g cm-3	2.301	2.301
Z	1	2
Mu (mm-1)	9.116	9.116
F000	1904.0	1904.0
F000'	1895.92	
h,k,lmax	12,19,34	12,19,34
Nref	17899	17895
Tmin,Tmax		0.610,0.619
Tmin'		

Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.619
AbsCorr = SPHERE

Data completeness= 1.000 Theta(max)= 30.508

R(reflections)= 0.0503(11836) wR2(reflections)= 0.1160(17895)

S = 1.023 Npar= 496

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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 10 Report
O13 O14 N1 N2 C25 C26 etc.
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 9.4 Ratio
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.05A From Br7 2.71 eA-3

Alert level C

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Sb2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.461 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.89A From Sb2 1.79 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85A From Br7 1.71 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.33A From Br8 1.69 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93A From Br8 1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.78A From Br7 -2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.39A From Br8 -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.66A From Br7 -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.57A From Br7 -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.82A From Br8 -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.60A From Sb2 -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.44A From Br8 -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.69A From Br8 -1.53 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ba2 1.15 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Sb1 1.15 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ba1 1.01 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24B -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30A -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H27D -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30D -0.51 eA-3

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.14 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 8 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br1 . 19.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br2 . 20.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br3 . 8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br4 . 6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br6 . 6.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O15 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C33 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33B Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H33C       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        18% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        33% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C26 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C27 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C29 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C30 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C32 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
              C27A     -H27E            1.555   1.555 ........     #   73 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         60 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1       (III)     .       2.83 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
23 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 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
24 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

Datablock 1 - ellipsoid plot