checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 4_18srv314

Bond precision: C-C = 0.0099 A Wavelength=0.71073

Cell: a=11.0794(6) b=19.5994(11) c=59.837(3)
alpha=90 beta=93.9088(15) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	12963.4(12)	12963.3(12)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	3(C49 H33), 3(Cl6 Sb), 2(C H2 Cl2)	Cl6 Sb 1-, 0.67(C H2 Cl2), C49 H33 1+
Sum formula	C149 H103 Cl22 Sb3	C49.67 H34.33 Cl7.33 Sb
Mr	3038.49	1012.82
Dx,g cm-3	1.557	1.557
Z	4	12
Mu (mm-1)	1.128	1.128
F000	6096.0	6096.0
F000'	6103.60	
h,k,lmax	13,23,71	13,23,71
Nref	22904	22893
Tmin,Tmax	0.835,0.968	0.772,0.984
Tmin'	0.695	

Correction method= # Reported T Limits: Tmin=0.772 Tmax=0.984
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 25.027

R(reflections)= 0.0724(18106) wR2(reflections)= 0.1483(22893)

S = 1.197 Npar= 1566

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

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PLAT031_ALERT_4_C Refined Extinction Parameter Within Range .....      3.071 Sigma
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          1 Check
            C51
PLAT213_ALERT_2_C Atom C1A             has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C2A             has ADP max/min Ratio .....        3.7 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 3  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        Cl7 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        Cl8 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        SbB Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        SbA Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C51 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl7      0.121 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl9A      0.155 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C51      -Cl9B           1.900 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0099 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H1A      ..H12A     .       1.98 Ang.
                                                    x,y,z  =      1_555 Check
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C49.67 H34.33 Cl7.33 Sb1
           Atom count from _chemical_formula_moiety:C49.67 H34.34 Cl7.34 Sb1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z   12
          From the CIF: _chemical_formula_sum  C49.67 H34.33 Cl7.33 Sb
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        596.04    596.00    0.04
          H        411.96    412.00   -0.04
          Cl        87.96     88.00   -0.04
          Sb        12.00     12.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         8 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       176 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ    Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.3333 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    104.12 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C50A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C50B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50C       Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H50D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl9A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl9B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51D       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )        33% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )        33% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C5A      -C14A     .       1.43 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl9B     ..C34B             3.22 Ang.
                                  1/2-x,-1/2+y,1/2-z  =      2_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl9B     ..C41B             3.25 Ang.
                                                    x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2B     ..Cl9A             2.99 Ang.
                                                    x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2B     ..Cl9B             3.23 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          6 Note
PLAT793_ALERT_4_G Model has Chirality at C16A        (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C16B        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C16C        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C17A        (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C17B        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C17C        (Centro SPGR)          R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for SbC       (V)       .       5.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for SbB       (V)       .       5.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for SbA       (V)       .       5.07 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1467 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  41 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  29 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 18/12/2021; check.def file version of 18/12/2021

Datablock 4_18srv314 - ellipsoid plot