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: I

Bond precision: Zn- O = 0.0130 A Wavelength=0.71070

Cell: a=4.0634(6) b=17.163(2) c=10.4699(13)
alpha=90 beta=91.024(11) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	730.06(16)	730.06(16)
Space group	?	?
Hall group		?
Moiety formula	Cl4 O7.61 Sb4 Zn3	?
Sum formula	Cl4 O7.61 Sb4 Zn3	Cl4 O7.61 Sb4 Zn3.61
Mr	946.77	986.60
Dx,g cm-3	2.154	4.487
Z	1	2
Mu (mm-1)	6.440	13.860
F000	422.9	882.0
F000’	422.15	
h,k,lmax	6,26,16	6,25,16
Nref	11624[5812]	22220
Tmin,Tmax		0.555,1.000
Tmin’		

Correction method= MULTI-SCAN

Data completeness= 3.82/1.91 Theta(max)= 33.640

R(reflections)= 0.0714(3537) wR2(reflections)= wR= 0.1404(22220)

S = 1.130 Npar= Npar = 362

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 A

SYMM004_ALERT_1_A _symmetry_equiv_pos_as_xyz loop is missing.
The symmetry equivalent positions in xyz.
The following tests will not be performed.
CELLZ_01,CHEMW_03,REFLT_03,SYMMG_01,SYMMG_02
GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.
GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -9.040
Test value = -5.100
DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
_refine_diff_density_max given = 9.130
Test value = 5.100

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.149

Alert level G

PLAT814_ALERT_5_G No Validation of (In)commensurate Structure CIFs Note

5 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock I - ellipsoid plot