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: C-C = 0.0040 A Wavelength=0.71075

Cell: a=13.8733(19) b=15.0486(18) c=14.7284(19)
alpha=90 beta=107.4300(17) gamma=90
Temperature: 135 K

	Calculated	Reported
Volume	2933.7(7)	2933.7(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H40 B4 Cl2 N24 O4 Yb2, 2(C H2 Cl2)	C42 H40 B4 Cl2 N24 O4 Yb2, 2(C H2 Cl2)
Sum formula	C44 H44 B4 Cl6 N24 O4 Yb2	C44 H44 B4 Cl6 N24 O4 Yb2
Mr	1575.05	1575.03
Dx,g cm-3	1.783	1.783
Z	2	2
Mu (mm-1)	3.506	3.506
F000	1540.0	1540.0
F000’	1540.62	
h,k,lmax	18,19,19	18,19,19
Nref	6723	6679
Tmin,Tmax	0.435,0.496	0.392,0.496
Tmin’	0.172	

Correction method= # Reported T Limits: Tmin=0.392 Tmax=0.496
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 27.490

R(reflections)= 0.0251(6002) wR2(reflections)= 0.0551(6679)

S = 1.050 Npar= 379

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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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl2      0.078 Check
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1       - C2       .       1.53 Ang.
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Alert level G

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PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1       -C3_a     .       1.44 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         87 Check
             O1   -C1   -YB1     1.555   1.555   1.555             39.41 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         93 Check
             O2   -C2   -YB1     1.555   1.555   1.555             39.11 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Yb1       (III)     .       3.26 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
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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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/12/2018; check.def file version of 11/12/2018

Datablock I - ellipsoid plot