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: 123

```
Bond precision:  C-C = 0.0392 A          Wavelength=0.71069

Cell:              a=19.503(5)      b=19.503(5)      c=18.892(5)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K

                Calculated                  Reported
Volume          7186(4)                     7186(3)
Space group     P 4/n                       P 4/n
Hall group      -P 4a                       -P 4a
Moiety formula  C152 H108 O25 Tb5, C Cl2    C152 H108 O25 Tb5, C Cl2
Sum formula     C153 H108 Cl2 O25 Tb5       C153 H108 Cl2 O25 Tb5
Mr              3211.94                     3211.94
Dx,g cm-3       1.484                       1.484
Z               2                           2
Mu (mm-1)       2.533                       2.533
F000            3170.0                      3170.0
F000'           3170.11
h,k,lmax        23,23,22                    23,23,22
Nref            6355                        6355
Tmin,Tmax       0.533,0.719                 0.533,0.719
Tmin'           0.463

Correction method= MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.000

R(reflections)= 0.0752( 3947)     wR2(reflections)= 0.2094( 6355)

S = 1.073                  Npar= 415
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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

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SHFSU01_ALERT_2_B  The absolute value of parameter shift to su ratio > 0.10
            Absolute value of the parameter shift to su ratio given   0.108
            Additional refinement cycles may be required.
PLAT080_ALERT_2_B Maximum Shift/Error ..........................       0.11
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          1 Report
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....        C33 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....         O9 Check
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.0392 Ang.
PLAT367_ALERT_2_B Long?  C(sp?)-C(sp?) Bond  C33    -   C50    ...       1.71 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C33    -   C36    ...       1.59 Ang.
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Alert level C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.36 Report
PLAT147_ALERT_1_C su on Symmetry Constrained Cell Angle(s) .......     Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          2
PLAT213_ALERT_2_C Atom C16             has ADP max/min Ratio .....        3.6 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        5.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O9     --  C33     ..        7.0 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O4     --  C6      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22    --  C23     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23    --  C28     ..       0.20 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C2 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C7 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C16 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C30 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C4 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C5 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C20 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         C98 Check
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C48    -   C49    ...       1.18 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        100 Ang3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         14 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     134.90 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =         33 Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C50    Che
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.22 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C Cl2
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        253 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   8 ALERT level B = A potentially serious problem, consider carefully
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 24 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
  8 ALERT type 4 Improvement, methodology, query or suggestion
  1 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*, 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 20/08/2014; check.def file version of 18/08/2014

Datablock 123 - ellipsoid plot