checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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 = 0.0111 A Wavelength=0.71073

Cell: a=47.9295(17) b=47.9295(17) c=13.1746(4)
alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	26210(2)	26210(2)
Space group	R -3 m	R -3 m
Hall group	-R 3 2"	-R 3 2"
Moiety formula	C29 H13 N O13 Tb Zn [+ solvent]	0.17(C522 H234 N18 O234 Tb18 Zn18)
Sum formula	C29 H13 N O13 Tb Zn [+ solvent]	C87 H39 N3 O39 Tb3 Zn3
Mr	807.72	2423.03
Dx,g cm-3	0.921	0.921
Z	18	6
Mu (mm-1)	1.651	1.651
F000	7074.0	7074.0
F000'	7079.59	
h,k,lmax	57,57,15	57,57,15
Nref	5407	5374
Tmin,Tmax	0.726,0.768	0.680,0.746
Tmin'	0.712	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.092

R(reflections)= 0.0711(3593) wR2(reflections)= 0.2441(5374)

S = 1.064 Npar= 226

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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Zn1 2.93 eA-3

Author Response: The large residual peak of 2.93 electrons per \%A^3^, located 0.29 \%A from the zinc atom, may be the result of residual absorption errors.

Alert level B

PLAT420_ALERT_2_B D-H Without Acceptor O1W --H1WA . Please Check

Author Response: Highly disordered solvent was located in this structure. Reflection contributions from this solvent were removed in the refinement. Thus no H bonding interactions were detected for O1W--H1WA and O1W--H1WB.

PLAT420_ALERT_2_B D-H Without Acceptor O1W --H1WB . Please Check

Author Response: Highly disordered solvent was located in this structure. Reflection contributions from this solvent were removed in the refinement. Thus no H bonding interactions were detected for O1W--H1WA and O1W--H1WB.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.156
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.156 Report
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Tb1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01108 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C6 - C8 . 1.53 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -11.548 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 28 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H1WB -0.32 eA-3

Alert level G

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: C87 H39 N3 O39 Tb3 Zn3
Atom count from _chemical_formula_moiety:C88.74 H39.78 N3.06 O39.78 Tb
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       3.00 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      12.34 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16B       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17B       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16        Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at       0.35 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         14% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C15      - C19      .        1.54 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1              77.7 Degree
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure         ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C16      --C17             1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C17B     --C18             2.00 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          40 Check
             C13  -C12  -C13B    1.555   1.555   1.555             27.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          43 Check
             C17  -C12  -C17B    1.555   1.555   1.555             25.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          51 Check
             C14  -C13  -C14B    1.555   1.555   1.555             26.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          58 Check
             C13  -C14  -C13B    1.555   1.555   1.555             27.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          69 Check
             C17B -C16  -C17     1.555   1.555   1.555             19.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          83 Check
             C17B -C17  -C16B    1.555   1.555   1.555             36.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          86 Check
             C16B -C17  -C16     1.555   1.555   1.555             21.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          98 Check
             C17  -C17B -C18     1.555   1.555   1.555             27.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         100 Check
             C16B -C17B -C16     1.555   1.555   1.555             23.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         107 Check
             C17B -C16B -C17     1.555   1.555   1.555             17.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         120 Check
             C14B -C13B -C14     1.555   1.555   1.555             25.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         127 Check
             C13B -C14B -C13     1.555   1.555   1.555             28.73 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         133 Check
             C14  -C15  -C14B    1.555   1.555   1.555             27.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         136 Check
             C16  -C15  -C16B    1.555   1.555   1.555             22.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         142 Check
             C17  -C18  -C17B    1.555   1.555   1.555             10.60 Deg.
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PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          7 Check
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        3 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        36% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        28 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         7 Info
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
57 **ALERT level G** = General information/check it is not something unexpected

3 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
11 ALERT type 3 Indicator that the structure quality may be low
38 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

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PUBL004_ALERT_1_A  The contact author’s name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. ’Acta Crystallographica Section C’
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
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7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

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 level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

```
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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 04/06/2020; check.def file version of 02/06/2020

Datablock I - ellipsoid plot