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 = 0.0367 A   Wavelength=0.71073

Cell: a=19.0949(11)   b=19.0949(11)   c=21.3112(13)
                alpha=90   beta=90   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	7770.4(10)	7770.4(10)
Space group	I 4 2 2	I 4 2 2
Hall group	I 4 2	I 4 2
Moiety formula	C80 H64 N32 S8 Zn4	C80 H64 N32 S8 Zn4
Sum formula	C80 H64 N32 S8 Zn4	C80 H64 N32 S8 Zn4
Mr	1991.67	1991.59
Dx,g cm-3	0.851	0.851
Z	2	2
Mu (mm-1)	0.754	0.754
F000	2032.0	2032.0
F000'	2036.63	
h,k,lmax	24,24,27	24,24,26
Nref	4183[2369]	4143
Tmin,Tmax	0.762,0.798	0.719,0.937
Tmin'	0.686	

Correction method= # Reported T Limits: Tmin=0.719 Tmax=0.937
AbsCorr = NUMERICAL

Data completeness= 1.75/0.99   Theta(max)= 26.802

R(reflections)= 0.1635(1419)   wR2(reflections)= 0.4430(4143)

S = 1.189   Npar= 142

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

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure   ! Info

🟠 Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
               Rint given   0.186
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ....   0.186 Report
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..   34% Check
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ....   0.8513 Check
PLAT082_ALERT_2_B High R1 Value ....   0.16 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ....   0.44 Report
PLAT230_ALERT_2_B Hirshfeld Test Diff for   N2   --C3   .   10.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for   N3   --C10   .   9.5 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference N2   --N3   0.26 Ang.
PLAT330_ALERT_2_B Large Average Phenyl C-C Dist C4   -C14   1.42 Ang.
PLAT332_ALERT_2_B Large Phenyl C-C Range   C4   -C14   0.35 Ang.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.03667 Ang.

🟡 Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
               The relevant atom site should be identified.
STRVA01_ALERT_4_C   Flack test results are ambiguous.
           From the CIF: _refine_ls_abs_structure_Flack   0.670
           From the CIF: _refine_ls_abs_structure_Flack_su   0.140
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   3.10 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density   2.27 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for   N1   --C1   .   6.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Zn1   --N2   0.22 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   S1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   N2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   N3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C8 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Zn1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C3 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C10 Check
PLAT368_ALERT_2_C Short C(sp2)-C(sp2) Bond C8   - C12   .   1.21 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C8   - C9   .   1.56 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor   N5   --H5A   Please Check
PLAT420_ALERT_2_C D-H Without Acceptor   N5   --H5B   Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   9.807 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.800 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .   0.67 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   7 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   5 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93A   From C14   2.21 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93A   From C14   1.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90A   From N5   0.44 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

⚪ Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   6 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.670 Note
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.20 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records   1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records   1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report

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PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)    293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)    293 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     87 Note
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ......      ! Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      12 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      8 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
  12 ALERT level B = A potentially serious problem, consider carefully
  26 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  28 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
  10 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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checkCIF publication errors

🔴 Alert level A

```
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.
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.
```

⚪ Alert level G

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PUBL017_ALERT_1_G The _publ_section_references section is missing or
          empty.
```

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   6 ALERT level A = Data missing that is essential or data in wrong format
   1 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_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: ...
;
_vrf_PLAT602_I
;
```

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PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
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 30/01/2018; check.def file version of 30/01/2018

Datablock I - ellipsoid plot