checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FJI-C8

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: FJI-C8

Bond precision: C-C = 0.0144 A Wavelength=1.54184

Cell: a=45.0598(4) b=45.0598(4) c=45.0598(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	91489(2)	91489(2)
Space group	F 41 3 2	F 41 3 2
Hall group	F 4d 2 3	F 4d 2 3
Moiety formula	C108 H36 N24 O50 Zn9	?
Sum formula	C108 H36 N24 O50 Zn9	C108 H36 N24 O50 Zn9
Mr	3058.12	3057.94
Dx,g cm-3	0.888	0.888
Z	16	16
Mu (mm-1)	1.499	1.499
F000	24352.0	24352.0
F000'	24205.89	
h,k,lmax	55,55,55	48,38,54
Nref	7684[4423]	6866
Tmin,Tmax	0.861,0.861	
Tmin'	0.861	

Correction method= Not given

Data completeness= 1.55/0.89 Theta(max)= 73.202

R(reflections)= 0.0845(2653) wR2(reflections)= 0.2972(6866)

S = 0.900 Npar= 288

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

PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C4 - C9 .. 1.60 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact O8 .. O9 .. 2.77 Ang.
PLAT990_ALERT_1_B Depricated RES file style based SQUEEZE job .... ! Note

---

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.297
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C9 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C2 -C7 1.35 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01437 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C10 - C11 .. 1.54 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C15 - C18 .. 1.53 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 10.345 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.268 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.584 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.235 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.368 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 243 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 87 %

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 19 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.14 Ratio
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 289 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 136 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 7 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 17 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

---

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

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_RFACR01_FJI-C8
;
PROBLEM: The value of the weighted R factor is > 0.25
RESPONSE: ...
;
_vrf_PLAT052_FJI-C8
;
PROBLEM: Info on Absorption Correction Method   Not Given     Please Do !
RESPONSE: ...
;
_vrf_PLAT084_FJI-C8
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.30 Report
RESPONSE: ...
;
_vrf_PLAT241_FJI-C8
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
RESPONSE: ...
;
_vrf_PLAT242_FJI-C8
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
RESPONSE: ...
;
_vrf_PLAT334_FJI-C8
;
PROBLEM: Small Average Benzene  C-C Dist. C2     -C7            1.35 Ang.
RESPONSE: ...
;
_vrf_PLAT341_FJI-C8
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............    0.01437 Ang.
RESPONSE: ...
;
_vrf_PLAT369_FJI-C8
;
PROBLEM: Long    C(sp2)-C(sp2) Bond  C10    -   C11    ..       1.54 Ang.
RESPONSE: ...
;
_vrf_PLAT906_FJI-C8
;
PROBLEM: Large K value in the Analysis of Variance ......     10.345 Check
RESPONSE: ...
;
_vrf_PLAT911_FJI-C8
;
PROBLEM: Missing # FCF Refl Between THmin & STh/L=  0.600        243 Report
RESPONSE: ...
;
```

```
_vrf_PLAT915_FJI-C8
;
PROBLEM: No Flack x Check Done: Low Friedel Pair Coverage         87 %
RESPONSE: ...
;
# end Validation Reply Form
```

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* or *IUCrData*, 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 11/08/2016; check.def file version of 04/08/2016

Datablock FJI-C8 - ellipsoid plot