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: exp_1c

Bond precision: C-C = 0.0163 A Wavelength=1.54184

Cell: a=9.9975(7) b=10.5491(7) c=11.4155(8)
alpha=95.125(5) beta=105.503(6) gamma=90.461(5)
Temperature: 150 K

	Calculated	Reported
Volume	1154.85(14)	1154.85(14)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C40 H30 I4 N2 O2 Zn2, 2(C H2 Cl2)	C40 H30 I4 N2 O2 Zn2, 2(C H2 Cl2)
Sum formula	C42 H34 Cl4 I4 N2 O2 Zn2	C42 H34 Cl4 I4 N2 O2 Zn2
Mr	1378.89	1378.85
Dx,g cm-3	1.983	1.983
Z	1	1
Mu (mm-1)	24.687	24.686
F000	656.0	656.0
F000’	654.69	
h,k,lmax	12,12,13	12,12,13
Nref	4439	4315
Tmin,Tmax	0.023,0.025	0.210,1.000
Tmin’	0.004	

Correction method= MULTI-SCAN

Data completeness= 0.972 Theta(max)= 70.810

R(reflections)= 0.0799(3851) wR2(reflections)= 0.2262(4315)

S = 1.078 Npar= Npar = 255

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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DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      4.370
           Test value =      3.975
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.972 Note
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       4.37 eA-3
PLAT213_ALERT_2_C Atom C5              has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C7              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C8              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.8 prolat
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C21 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        4.0 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0163 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C9     -   C10    ...       1.55 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.16 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I1     --  Zn1_a   ..        9.4 su
```

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

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

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 05/02/2014; check.def file version of 05/02/2014

Datablock exp_1c - ellipsoid plot