

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=10.426(3) b=11.235(3) c=13.101(3)
 alpha=110.067(3) beta=112.286(3) gamma=93.936(3)
Temperature: 98 K

	Calculated	Reported
Volume	1298.4(6)	1298.4(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H46 N8 O4 S10 Zn2, 2(C3 H7 N O)	C30 H46 N8 O4 S10 Zn2, 2(C3 H7 N O)
Sum formula	C36 H60 N10 O6 S10 Zn2	C36 H60 N10 O6 S10 Zn2
Mr	1180.42	1180.28
Dx,g cm-3	1.510	1.509
Z	1	1
Mu (mm-1)	1.377	1.377
F000	614.0	614.0
F000'	615.95	
h,k,lmax	12,13,16	12,13,16
Nref	5104	5058
Tmin,Tmax	0.726,0.933	0.813,1.000
Tmin'	0.702	

Correction method= MULTI-SCAN

Data completeness= 0.991

Theta(max)= 26.000

R(reflections)= 0.0364(4809)

wR2(reflections)= 0.0906(5058)

S = 0.952

Npar= 302

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

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C15 - C15_a ...	1.54 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 	1
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	41

PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L=	0.600	3
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		2
PLAT975_ALERT_2_C Positive Residual Density at 1.08Å from Ol	.	0.65 eÅ ⁻³



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		6
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF		?
PLAT153_ALERT_1_G The su's on the Cell Axes are Equal	0.00300 Ang.	
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal	0.00300 Deg.	
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp ²)-Methyl Moiety		C6
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		2
C3 H7 N O		
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints		3

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

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

checkCIF publication errors



Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

0 **ALERT level A** = Data missing that is essential or data in wrong format
2 **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 you wish to submit your CIF for publication in Acta Crystallographica Section C or E, 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 21/12/2011; check.def file version of 16/12/2011

Datablock I - ellipsoid plot

