

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_4

Bond precision: C-C = 0.0065 Å Wavelength=0.71073
Cell: a=7.5823(19) b=6.863(5) c=21.039(14)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1094.8(11)	1094.8(12)
Space group	P m n n	Pmnn
Hall group	-P 2n 2	?
Moiety formula	C10 H12 N O5 Zn	?
Sum formula	C10 H12 N O5 Zn	C10 H12 N O5 Zn
Mr	291.60	291.58
Dx,g cm-3	1.769	1.769
Z	4	4
Mu (mm-1)	2.252	2.252
F000	596.0	596.0
F000'	597.41	
h,k,lmax	9,8,27	9,8,27
Nref	1355	1319
Tmin,Tmax	0.947,0.956	
Tmin'	0.798	

Correction method= Not given

Data completeness= 0.973 Theta(max)= 27.530

R(reflections)= 0.0462(965) wR2(reflections)= 0.0924(1319)

S = 1.080 Npar= 92

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full	Low	0.973
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds	0.0065 Ang

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	3
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT128_ALERT_4_G	Alternate Setting of Space-group Pnnm	Pnnm
PLAT194_ALERT_1_G	Missing _cell_measurement_reflms_used datum	?
PLAT195_ALERT_1_G	Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_G	Missing _cell_measurement_theta_min datum	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.19 Ratio
PLAT793_ALERT_4_G	The Model has Chirality at C2 (Verify)	S
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	1

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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 21/12/2011; check.def file version of 16/12/2011

Datablock compound_4 - ellipsoid plot

