

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P-1_a

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: P-1_a

Bond precision: C-C = 0.0039 Å Wavelength=0.63000

Cell: a=10.941(2) b=12.674(3) c=14.043(3)
 alpha=100.78(3) beta=101.10(3) gamma=108.21(3)
Temperature: 200 K

	Calculated	Reported
Volume	1750.2(8)	1750.3(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C30.89 H27.42 N3.63 O7.63 Zn1.50), 2.738(C3 H7 N O)	?
Sum formula	C70 H74 N10 O18 Zn3	C70 H74 N10 O18 Zn3
Mr	1539.56	1539.50
Dx, g cm ⁻³	1.461	1.461
Z	1	1
Mu (mm ⁻¹)	0.793	0.793
F000	798.0	798.0
F000'	799.16	
h,k,lmax	15,17,19	15,17,19
Nref	10410	9774
Tmin,Tmax	0.828,0.904	0.548,0.906
Tmin'	0.505	

Correction method= # Reported T Limits: Tmin=0.548 Tmax=0.906
AbsCorr = EMPIRICAL

Data completeness= 0.939 Theta(max)= 26.500

R(reflections)= 0.0533(6570)	wR2(reflections)= 0.1648(9774)
S = 1.008	Npar= 571

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

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.956 Why?

Author Response: Since the Pohang Accelerator Laboratory 2D Beamline goniostat has only one omega-axis, diffrn_measured_fraction_theta_full is not fully covered as 0.956, especially for the low symmetry such as triclinic system. As this is an inherent problem, other command and option were not helpful to improve the completeness.



Alert level C

PLAT213_ALERT_2_C	Atom C5B	has ADP max/min Ratio	3.8	oblate
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		02	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	01B	0.101	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	03B	0.117	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.808	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	278	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1	Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H7A		-0.39	eA-3



Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.			
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		30	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		11	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..		0.86	mm
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.63000	Ang.
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.03	Degree
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		3	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		3	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		18	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records		18	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		6	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		6	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Zn2	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H25B ..H2B3	2.11	Ang.
		1-x,1-y,1-z =	2_666	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		36	Note

PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	17.27 Deg.
ZN2 -N1 -ZN2 1_555 1_555 2_766 	# 43 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	17.57 Deg.
ZN2 -N2 -ZN2 1_555 1_555 2_766 	# 49 Check	
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	1 Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	280 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	357 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6 Info
PLAT984_ALERT_1_G	The Zn-f' = 0.3273 Deviates from the B&C-Value	0.3261 Check
PLAT985_ALERT_1_G	The Zn-f" = 1.1646 Deviates from the B&C-Value	1.1614 Check

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

5 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
 7 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 3 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* 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.

