

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB3

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: MAB3

Bond precision: C-C = 0.0043 A

Wavelength=0.71075

Cell: a=9.3681(2) b=10.6910(2) c=19.2746(4)
 alpha=82.954(2) beta=76.156(2) gamma=68.655(2)
Temperature: 100 K

	Calculated	Reported
Volume	1744.44(7)	1744.44(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C3 H17 B12 N2 O24 Zn), 3(C3 H12 N2), 14(H2 O)	C3 H17 B12 N2 O24 Zn, 7(H2 O), 1.5(C3 H12 N2)
Sum formula	C15 H98 B24 N10 O62 Zn2	C7.50 H49 B12 N5 O31 Zn
Mr	1801.25	900.60
Dx,g cm-3	1.715	1.715
Z	1	2
Mu (mm-1)	0.821	0.821
F000	934.0	934.0
F000'	935.20	
h,k,lmax	12,13,25	12,13,25
Nref	7973	7958
Tmin,Tmax	0.871,0.936	0.910,1.000
Tmin'	0.870	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 27.484

R(reflections)= 0.0425(7654)

wR2(reflections)= 0.1053(7958)

S = 1.191

Npar= 590

```
test-name ALERT alert-type alert-level.
```

🚨 **Alert level B**

PLAT420_ALERT 2 B D-H Without Acceptor O34 --H34B . Please Check

```
PLAT417_ALERT_2_C Short Inter D-H..H-D      H32A       ..H34B     .          2.12 Ang.  
x,y,z =           1 555 Check
```

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	41	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.38	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT300_ALERT_4_G	Atom Site Occupancy of N21 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N22 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21D Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21E Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22D Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22E Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 9)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 10)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 11)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 12)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	8.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 9	1.57	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 10	1.64	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 11	1.42	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 12	1.36	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	17	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	10	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	12	Note
	H2 O		
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.93	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
30 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* 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 18/02/2019; check.def file version of 18/02/2019

