

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0045 Å	Wavelength=1.54178	
Cell:	a=9.9347 (14)	b=23.521 (3)	c=10.5889 (15)
	alpha=90	beta=93.195 (4)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	2470.5 (6)	2470.5 (6)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C26 H26 N4 O4 Zn	?
Sum formula	C26 H26 N4 O4 Zn	C26 H26 N4 O4 Zn
Mr	523.90	523.88
Dx, g cm ⁻³	1.409	1.409
Z	4	4
Mu (mm ⁻¹)	1.709	1.709
F000	1088.0	1088.0
F000'	1084.74	
h, k, l _{max}	11, 28, 12	11, 28, 12
Nref	4534 [2274]	4216
Tmin, Tmax	0.556, 0.774	0.537, 0.753
Tmin'	0.497	

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Correction method= # Reported T Limits: Tmin=0.537 Tmax=0.753
AbsCorr = MULTI-SCAN
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Data completeness= 1.85/0.93 Theta (max)= 68.452

R(reflections)= 0.0281(4208)	wR2(reflections)= 0.0725(4216)
S = 0.831	Npar= 319

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

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.03	Note
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	01	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N2 --H2A .	Please	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	23	Report
	0 4 0, 1 7 0, 2 10 0, 1 5 1, -1 9 1, -1 11 1,		
	-1 13 1, 0 0 2, 1 1 2, 0 2 2, -1 5 2, 0 10 2,		
	2 10 2, -1 11 2, 0 4 3, -1 9 3, -2 12 3, 4 0 4,		
	2 4 4, 0 0 6, 2 0 6, 0 0 8, -4 2 12,		



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
	H2A H2B H4A H4B		
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 --O1 .	21.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 --O2 .	13.2	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.83	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
	0 2 0,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	9	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	9	Note
	-1 5 2, -2 12 3, -1 11 2, -1 9 3, 0 4 3, 0 4 0,		
	-1 -7 0, -4 2 12, -1 7 0,		
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.67	Note
	Predicted wR2: Based on SigI**2 2.72 or SHELX Weight	9.07	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
2 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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.

