

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Zn2tdpd2pyz2-100K

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: Zn2tdpd2pyz2-100K

Bond precision:	C-C = 0.0018 A	Wavelength=0.71075	
Cell:	a=12.0699(3)	b=7.11859(17)	c=18.4918(5)
	alpha=90	beta=98.7958(9)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1570.14(7)	1570.14(7)	
Space group	P 2/n	P 1 2/n 1	
Hall group	-P 2yac	-P 2yac	
Moiety formula	C16 H4 N10 O4 Zn, C4 H12 N2 O4 Zn, 6(H2 O)	C20 H28 N12 O14 Zn2	
Sum formula	C20 H28 N12 O14 Zn2	C20 H28 N12 O14 Zn2	
Mr	791.32	791.32	
Dx,g cm-3	1.674	1.674	
Z	2	2	
Mu (mm-1)	1.612	1.613	
F000	808.0	808.0	
F000'	809.49		
h,k,lmax	15,9,23	15,9,23	
Nref	3601	3591	
Tmin,Tmax	0.623,0.851	0.623,0.851	
Tmin'	0.610		

Correction method= # Reported T Limits: Tmin=0.623 Tmax=0.851
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.465

R(reflections)= 0.0213(3370) wR2(reflections)= 0.0583(3601)

S = 1.131 Npar= 260

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

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	I	88 %Fit
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1 Check



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1 Info
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C3 --C5 .		6.6 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C4 --C6 .		6.5 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .		2.01 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn2 (II) .		2.00 Info
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		6 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3 Info

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- 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
11 **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
2 ALERT type 3 Indicator that the structure quality may be low
1 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.

