

checkCIF/PLATON report

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

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: sxt12_0m

Bond precision:	C-C = 0.0051 A	Wavelength=0.71073
Cell:	a=20.214(2) b=14.0472(17) c=13.9552(16)	
	alpha=90 beta=113.863(2) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	3623.8(7)	3623.8(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C21 H12 N3 O6 Zn	C21 H12 N3 O6 Zn
Sum formula	C21 H12 N3 O6 Zn	C21 H12 N3 O6 Zn
Mr	467.73	467.71
Dx,g cm-3	1.715	1.715
Z	8	8
Mu (mm-1)	1.405	1.405
F000	1896.0	1896.0
F000'	1899.11	
h,k,lmax	29,20,20	27,20,20
Nref	5919	5730
Tmin,Tmax	0.845,0.869	0.632,0.746
Tmin'	0.845	

Correction method= # Reported T Limits: Tmin=0.632 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.968 Theta(max)= 31.267

R(reflections)= 0.0562(3663) wR2(reflections)= 0.1771(5730)

S = 1.064 Npar= 292

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**

PLAT213_ALERT_2_C	Atom O6	has ADP max/min Ratio	3.2	prolat
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N3 --C8 .	6.5	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N3 --C9 .	6.0	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N3	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C20	Check	
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note	
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N3 --H3 .	Please	Check

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report	
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c	I2/a	Note
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report	
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn16 --C12 .	7.2	s.u.	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note	
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.7	Low	
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units	

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
2 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.

