

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: exp_1a

Bond precision:	C-C = 0.0095 A	Wavelength=1.54184	
Cell:	a=21.582(4)	b=10.6678(12)	c=23.718(3)
	alpha=90	beta=122.12(2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	4624.8(15)	4625.1(12)	
Space group	C 2/c	C 2/c	
Hall group	-C 2yc	?	
Moiety formula	C40 H30 Cl4 N2 O2 Zn2, 2(C H Cl3)	C40 H30 Cl4 N2 O2 Zn2, 2(C H Cl3)	
Sum formula	C42 H32 Cl10 N2 O2 Zn2	C42 H32 Cl10 N2 O2 Zn2	
Mr	1081.98	1081.98	
Dx,g cm-3	1.554	1.554	
Z	4	4	
Mu (mm-1)	6.896	6.895	
F000	2176.0	2176.0	
F000'	2181.85		
h,k,lmax	26,13,29	26,12,28	
Nref	4450	4339	
Tmin,Tmax	0.332,0.408	0.520,1.000	
Tmin'	0.251		

Correction method= MULTI-SCAN

Data completeness= 0.975 Theta(max)= 70.700

R(reflections)= 0.0561(2910) wR2(reflections)= 0.1923(4339)

S = 1.032 Npar= Npar = 265

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	Low	0.975	Note
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of			C21	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0095	Ang.

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF		Please	Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT	Unusually Large.		0.10	Why ?
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as			mixed	
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by	...		3	Units
PLAT158_ALERT_4_G	The Input Unitcell is NOT Standard/Reduced		Please	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)		293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)		293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1	-- Cl1_a	..	8.0	su
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	Cl4	.. Cl4	.	3.32 Ang.

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
1 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock exp_1a - ellipsoid plot

