

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) d437

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: d437

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: a=9.067(1) b=11.7201(13) c=12.4367(14)
 alpha=91.649(9) beta=108.557(10) gamma=104.506(10)
Temperature: 228 K

	Calculated	Reported
Volume	1204.4(3)	1204.4(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H46 Cl2 N4 O16 Zn4	C42 H46 Cl2 N4 O16 Zn4
Sum formula	C42 H46 Cl2 N4 O16 Zn4	C42 H46 Cl2 N4 O16 Zn4
Mr	1195.29	1195.21
Dx,g cm-3	1.648	1.648
Z	1	1
Mu (mm-1)	2.151	2.151
F000	608.0	608.0
F000'	609.67	
h,k,lmax	11,14,15	11,14,15
Nref	4748	4729
Tmin,Tmax	0.603,0.665	0.892,1.000
Tmin'	0.591	

Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 26.020

R(reflections)= 0.0441(3459) wR2(reflections)= 0.1167(4729)

S = 1.044 Npar= 312

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

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min)	Range	5.9	Ratio
PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	6.2	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C20	--	C21	..	0.21 Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for			07	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for			C17	Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.0073	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C19 - C20	...	1.43 Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on	AtSite	6	Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	Please	Do !
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note

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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
 - 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 3 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 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
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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*, 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 20/08/2014; check.def file version of 18/08/2014

Datablock d437 - ellipsoid plot

