

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: a_a_sq

Bond precision: C-C = 0.0152 A

Wavelength=0.71073

Cell: a=10.458(2) b=14.957(3) c=15.260(3)
 alpha=117.530(5) beta=98.114(6) gamma=96.867(6)
Temperature: 273 K

	Calculated	Reported
Volume	2048.6(7)	2048.6(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H32 Ca N12 O11, C6 H5 N O3, Cl4 Zn [+ solvent]	Cl4 Zn, C21 H32 Ca N12 O11, C6 H5 N O3
Sum formula	C27 H37 Ca Cl4 N13 O14 Zn [+ solvent]	C27 H37 Ca Cl4 N13 O14 Zn
Mr	1014.97	1014.94
Dx, g cm ⁻³	1.645	1.645
Z	2	2
Mu (mm ⁻¹)	1.065	1.065
F000	1040.0	1040.0
F000'	1042.62	
h,k,lmax	12,17,18	12,17,18
Nref	7223	6925
Tmin,Tmax	0.847,0.880	0.589,0.746
Tmin'	0.766	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.959

Theta(max)= 24.999

R(reflections)= 0.0847(4830)

wR2(reflections)= 0.2565(6925)

S = 1.046

Npar= 546

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 B

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full value Low	.	0.959	Why?
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds	0.01515	Ang.
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O7 --H7A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O9 --H9A	.	Please Check

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.26	Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 O	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	5.3	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O14 --N13	0.21	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Ca1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C22	Check

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	11	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ			Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		18.18	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	273	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	273	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		79	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II)	.	1.95	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

4 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
4 ALERT type 3 Indicator that the structure quality may be low
3 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.

PLATON version of 03/06/2021; check.def file version of 02/06/2021

