

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: sun-16

Bond precision: C-C = 0.0060 A

Wavelength=0.71073

Cell: a=9.3223(5) b=13.1795(5) c=16.5396(10)
 alpha=92.650(4) beta=105.391(5) gamma=102.938(4)
Temperature: 293 K

	Calculated	Reported
Volume	1897.38(18)	1897.38(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H29 N7 O11 Zn2, C3 H7 N O, H O, H2 O	C28 H29 N7 O11 Zn2, C3 H7 N O, H O, H2 O
Sum formula	C31 H39 N8 O14 Zn2	C31 H40 N8 O14 Zn2
Mr	878.48	879.45
Dx,g cm-3	1.538	1.539
Z	2	2
Mu (mm-1)	1.340	1.340
F000	906.0	908.0
F000'	907.54	
h,k,lmax	11,15,19	11,15,19
Nref	6672	6669
Tmin,Tmax	0.676,0.725	
Tmin'	0.645	

Correction method= Not given

Data completeness= 1.000

Theta(max)= 24.998

R(reflections)= 0.0432(4816)

wR2(reflections)= 0.0956(6669)

S = 1.026

Npar= 509

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O10	--C27	.	8.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C27	--C28	.	9.5 s.u.

Alert level C

PLAT018_ALERT_1_C	_diffn_measured_fraction_theta_max	.NE.	*_full		! Check
PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ		Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by	..	0.97	Check
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given			Please Do !
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min)	Range	3.9	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min)	Range	4.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			05	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			011	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			Zn1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C12	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C27	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of			N8	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H13A	..H14B	2.13	Ang.

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C31 H40 N8 O14 Zn2
Atom count from _chemical_formula_moiety: C31 H39 N8 O14 Zn2

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C31 H40 N8 O14 Zn2
Atom count from the _atom_site data: C31 H39 N8 O14 Zn2

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C31 H40 N8 O14 Zn2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	62.00	62.00	0.00
H	80.00	78.00	2.00
N	16.00	16.00	0.00
O	28.00	28.00	0.00
Zn	4.00	4.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF		Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C8 - C9_e	1.50	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II)	1.94	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn2 (II)	1.96	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	1	Info

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

11 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
5 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.

