

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: wang1

Bond precision: C-C = 0.0119 A

Wavelength=0.71073

Cell: a=10.0751(6) b=10.2040(5) c=11.4148(5)
 alpha=100.519(4) beta=95.060(4) gamma=106.233(5)
Temperature: 293 K

	Calculated	Reported
Volume	1095.68(10)	1095.68(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H20 N6 O4 Zn, H2 O	C22 H20 N6 O4 Zn, H2 O
Sum formula	C22 H22 N6 O5 Zn	C22 H22 N6 O5 Zn
Mr	515.85	515.85
Dx,g cm-3	1.564	1.564
Z	2	2
Mu (mm-1)	1.169	1.169
F000	532.0	532.0
F000'	532.76	
h,k,lmax	11,12,13	11,12,13
Nref	3867	3860
Tmin,Tmax	0.701,0.747	0.787,0.845
Tmin'	0.673	

Correction method= # Reported T Limits: Tmin=0.787 Tmax=0.845
AbsCorr = EMPIRICAL

Data completeness= 0.998

Theta(max)= 25.000

R(reflections)= 0.0882(3115)

wR2(reflections)= 0.2773(3860)

S = 1.087

Npar= 307

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

PLAT220_ALERT_2_B	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min) Range	7.0	Ratio
PLAT220_ALERT_2_B	Non-Solvent	Resd 1	N	Ueq(max)/Ueq(min) Range	6.5	Ratio
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C7	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check	
PLAT411_ALERT_2_B	Short Inter H...H Contact	H7	..H7	1.88	Ang.	
PLAT420_ALERT_2_B	D-H Without Acceptor	O8	--H8A	Please	Check	
PLAT420_ALERT_2_B	D-H Without Acceptor	O8	--H8B	Please	Check	

🟢 Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report	
PLAT213_ALERT_2_C	Atom C7	has ADP max/min Ratio	3.3	prolat	
PLAT213_ALERT_2_C	Atom C9	has ADP max/min Ratio	3.1	prolat	
PLAT222_ALERT_3_C	Non-Solv. Resd 1	H Uiso(max)/Uiso(min) Range	7.7	Ratio	
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N1 --C22	6.2	s.u.	
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N16 --C28	6.4	s.u.	
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Zn1 --O1	7.0	s.u.	
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Zn1 --N8	6.0	s.u.	
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Zn1 --N9	6.0	s.u.	
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Zn1 --O2_a	8.5	s.u.	
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C2	Check	
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C3	Check	
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C9	Check	
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N7	Check	
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N8	Check	
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N9	Check	
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N10	Check	
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C28	Check	
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note	
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C5 -C13	1.36	Ang.	
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.01194	Ang.	
PLAT420_ALERT_2_C	D-H Without Acceptor	N1 --H1A	Please	Check	
PLAT420_ALERT_2_C	D-H Without Acceptor	N1 --H1B	Please	Check	

🟠 Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info	
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report	
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.19	Report	
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check	(K)
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check	(K)
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.12	Ratio	
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II)	1.53	Info	

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
7 **ALERT level B** = A potentially serious problem, consider carefully
23 **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

- 3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
28 **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
4 **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* 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.

