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: new_sq

```
Bond precision:  C-C = 0.0127 A          Wavelength=0.70000

Cell:              a=30.315(4)      b=30.315(4)      c=34.474(7)
                   alpha=90         beta=90          gamma=90
Temperature:       233 K
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	Calculated	Reported
Volume	31682(11)	31682(11)
Space group	P 4/m n c	P 4/m n c
Hall group	-P 4 2n	-P 4 2n
Moiety formula	2(C79 H41.60 N7.40 O17.90 Zn5.50) [+ solvent]	?
Sum formula	C158 H83.20 N14.80 O35.80 Zn11 [+ solvent]	C158 H83.20 N14.80 O35.80 Zn11
Mr	3480.89	3480.66
Dx,g cm-3	0.730	0.730
Z	4	4
Mu (mm-1)	0.821	0.821
F000	7004.8	7005.0
F000’	7020.42	
h,k,lmax	34,34,39	34,34,39
Nref	12532	12473
Tmin,Tmax	0.821,0.863	0.714,0.866
Tmin’	0.697	

```
Correction method= # Reported T Limits: Tmin=0.714 Tmax=0.866
AbsCorr = MULTI-SCANS

Data completeness= 0.995          Theta(max)= 23.500

R(reflections)= 0.1200( 10747)    wR2(reflections)= 0.4320( 12473)

S = 2.059                 Npar= 511
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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

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THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5696
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................       0.43 Report
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        O2W Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         N4 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Zn5 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
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Alert level C

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ABSMU01_ALERT_1_C  The ratio of given/expected absorption coefficient lies
              outside the range 0.99 <> 1.01
           Calculated value of mu =     0.856
           Value of mu given      =     0.821
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      2.059
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 0.71065-0.71075
           Wavelength given =    0.70000
PLAT082_ALERT_2_C High R1 Value ..................................       0.12 Report
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ..............       2.06 Check
PLAT213_ALERT_2_C Atom O4              has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom N4              has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C14             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C19             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C31             has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C32             has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C33             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C35             has ADP max/min Ratio .....        3.2 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       3.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1   O   Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O5 Check
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         C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C17 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C32 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C33 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zn2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N1P 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        C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C29 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01271 Ang.
PLAT368_ALERT_2_C Short   C(sp2)-C(sp2) Bond  C27    -   C27_k  ..       1.20 Ang.
PLAT369_ALERT_2_C Long    C(sp2)-C(sp2) Bond  C18    -   C34_a  ..       1.55 Ang.
PLAT731_ALERT_1_C Bond    Calc   1.549(14), Rep     1.55(7) ......          5 su-Rat
             C34  -C18         1.555   6.465 .....      #   77 Check
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Alert level G

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ABSTY01_ALERT_1_G  Extra text has been found in the _exptl_absorpt_correction_type
           field, which should be only a single keyword. A literature
           citation should be included in the _exptl_absorpt_process_details
           field.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        14 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.20 Report
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka    0.70000 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         3 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         4 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Zn4     is Constrained at       0.55 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Zn3     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1P     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2P     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1P     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2P     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7P     is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8P     is Constrained at       0.45 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..         9% Note
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C3P    -   C3P_h  ..       1.53 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        150 Check
             ZN4  -O2   -ZN3     1.555   1.555   1.555             28.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        154 Check
             ZN3  -O4   -ZN4     1.555   1.555   1.555             20.91 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        158 Check
             ZN4  -O6   -ZN3     1.555   1.555   1.555             22.01 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        192 Check
             ZN4  -O2W  -ZN3     1.555   1.555   1.555             29.88 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        153 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
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 0 ALERT level A = Most likely a serious problem - resolve or explain
12 ALERT level B = A potentially serious problem, consider carefully
42 ALERT level C = Check. Ensure it is not caused by an omission or oversight
39 ALERT level G = General information/check it is not something unexpected

 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
52 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
30 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* 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 13/08/2017; check.def file version of 27/07/2017

Datablock new_sq - ellipsoid plot