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

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Bond precision:  C-C = 0.0120 A          Wavelength=0.70000

Cell:              a=30.344(4)      b=30.344(4)      c=34.461(7)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
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	Calculated	Reported
Volume	31730(11)	31731(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	0.729	0.729
Z	4	4
Mu (mm-1)	0.819	0.819
F000	7004.8	7005.0
F000’	7020.42	
h,k,lmax	35,35,40	35,35,40
Nref	13300	13244
Tmin,Tmax	0.822,0.863	0.714,0.867
Tmin’	0.697	

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Correction method= # Reported T Limits: Tmin=0.714 Tmax=0.867
AbsCorr = MULTI-SCANS

Data completeness= 0.996          Theta(max)= 23.999

R(reflections)= 0.1111( 10344)    wR2(reflections)= 0.3992( 13244)

S = 1.731                 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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.40 Report
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 C16 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C33 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 C32 Check

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Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies outside the range 0.99 <> 1.01
Calculated value of mu = 0.854
Value of mu given = 0.819
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
THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5810
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT213_ALERT_2_C Atom C21 has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 5.2 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 O2 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 O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N2 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 C8 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 C25 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 C15 Check
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 C22 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 C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01205 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C5 - C6 .. 1.53 Ang.
PLAT731_ALERT_1_C Bond Calc 1.482(13), Rep 1.48(7) ..... 5 su-Rat
C27 -C35 1.555 6.565 ..... # 67 Check

Alert level G

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.

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 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.
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
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            26.34 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        154 Check
             ZN3  -O4   -ZN4     1.555   1.555   1.555            19.03 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        158 Check
             ZN4  -O6   -ZN3     1.555   1.555   1.555            20.98 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        192 Check
             ZN4  -O2W  -ZN3     1.555   1.555   1.555            27.57 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         44 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
7 **ALERT level B** = A potentially serious problem, consider carefully
31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
35 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
28 ALERT type 4 Improvement, methodology, query or suggestion
1 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 27/03/2017; check.def file version of 24/03/2017

Datablock new_sq - ellipsoid plot