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: stock17

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Bond precision:  C-C = 0.0109 A          Wavelength=0.71073

Cell:            a=9.0934(12)     b=31.653(3)        c=16.281(2)
                 alpha=90         beta=136.39(3)     gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	3232.3(19)	3232.2(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C21 H24 N9 P S Zn), 4(ClO4), 3(C2 H3 N)	C21 H24 N9 P S Zn 2+, 2(ClO4 1-), 1.5(C2 H3 N)
Sum formula	C48 H57 Cl4 N21 O16 P2 S2 Zn2	C24 H28.50 Cl2 N10.50 O8 P S Zn
Mr	1582.79	791.37
Dx,g cm-3	1.626	1.626
Z	2	4
Mu (mm-1)	1.104	1.104
F000	1620.0	1620.0
F000’	1623.78	
h,k,lmax	11,39,20	11,38,20
Nref	6341	6322
Tmin,Tmax	0.722,0.789	0.703,0.834
Tmin’	0.606	

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Correction method= # Reported T Limits: Tmin=0.703 Tmax=0.834
AbsCorr = ANALYTICAL

Data completeness= 0.997          Theta(max)= 25.999

R(reflections)= 0.0699( 5266)     wR2(reflections)= 0.1680( 6322)

S = 1.109                 Npar= 466
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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 C

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01087 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT012_ALERT_1_G No _shelx_res_checksum found in CIF ..... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 12.71 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c P21/n Note
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 7 Units
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 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl10 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl20 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N30 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32C is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N40 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42C is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N50 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C51 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52C is Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4).. 100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5).. 100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6).. 100 % Note
PLAT432_ALERT_2_G Short Inter X...Y Contact O21 .. C52 .. 2.98 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O23 .. C2 .. 2.95 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 18 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
Cl O4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 5 Note
C2 H3 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 6 Note
C2 H3 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 75 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 Note

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

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  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
 31 ALERT type 4 Improvement, methodology, query or suggestion
  0 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 27/03/2017; check.def file version of 24/03/2017

Datablock stock17 - ellipsoid plot