checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pvl632_a_sq

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: pvl632_a_sq

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Bond precision:   C-C = 0.0041 A          Wavelength=0.71073

Cell:             a=13.3256(3)     b=25.4765(6)         c=25.8209(7)
                  alpha=90         beta=104.918(1)      gamma=90
Temperature:      150 K
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	Calculated	Reported
Volume	8470.5(4)	8470.5(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H14 N8 O4 S Zn, C3 H7 N O [+ solvent]	?
Sum formula	C27 H21 N9 O5 S Zn [+ solvent]	C27 H21 N9 O5 S Zn
Mr	648.98	648.98
Dx,g cm-3	1.527	1.526
Z	12	12
Mu (mm-1)	0.999	0.999
F000	3984.0	3979.0
F000'	3990.25	
h,k,lmax	19,36,36	19,36,36
Nref	25870	25841
Tmin,Tmax	0.887,0.932	0.652,0.742
Tmin'	0.771	

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Correction method= # Reported T Limits: Tmin=0.652 Tmax=0.742
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 30.518
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R(reflections)= 0.0563(17090)

wR2(reflections)= 0.1417(25841)

S = 1.028 Npar= 1205

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

PLAT213_ALERT_2_C Atom N2 has ADP max/min Ratio ..... 3.8 prolat
PLAT213_ALERT_2_C Atom N3 has ADP max/min Ratio ..... 4.0 prolat
PLAT213_ALERT_2_C Atom O2 has ADP max/min Ratio ..... 3.2 prolat
PLAT215_ALERT_3_C Disordered S2' has ADP max/min Ratio ..... 3.2 Note
PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 3 O Ueq(max)/Ueq(min) Range 3.8 Ratio
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 N3 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N28 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.7 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.4 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.876 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.99A From O2 1.28 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82A From O14 0.54 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.84A From O2 -0.51 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.94 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of S2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S2' Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O17 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C81 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C181 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C82 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C180 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H81A Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H81B Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H81C Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H181 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18C Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H82 Constrained at 0.4 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 60% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C76 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H79A ..H181 . 2.01 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact S2' ..C45 3.25 Ang.
1-x,1-y,1-z = 3_666 Check

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PLAT432_ALERT_2_G Short Inter X...Y Contact  O1       ..C7              2.92 Ang.
                                                    x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        288 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.93 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       1.91 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn3       (II)      .       1.93 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         23 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        4.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
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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
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
35 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
23 ALERT type 4 Improvement, methodology, query or suggestion
4 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 13/07/2021; check.def file version of 13/07/2021

Datablock pvl632_a_sq - ellipsoid plot