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: 30_sq

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Bond precision:  C-C = 0.0058 A          Wavelength=0.71073

Cell:            a=7.8033(4)    b=30.0645(18)      c=20.5938(10)
                 alpha=90       beta=93.545(4)     gamma=90
Temperature:     293 K
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	Calculated	Reported
Volume	4822.1(4)	4822.1(4)
Space group	I 2/c	I 2/c
Hall group	-I 2yc	-I 2yc
Moiety formula	C36 H34 Er N4 O14 Zn2, C2 H3 O2 [+ solvent]	C36 H34 Er N4 O14 Zn2, C2 H3 O2
Sum formula	C38 H37 Er N4 O16 Zn2 [+ solvent]	C38 H37 Er N4 O16 Zn2
Mr	1103.76	1103.71
Dx,g cm-3	1.520	1.520
Z	4	4
Mu (mm-1)	2.777	2.777
F000	2196.0	2196.0
F000’	2198.24	
h,k,lmax	10,40,27	10,40,25
Nref	6327	5715
Tmin,Tmax	0.519,0.574	0.560,0.610
Tmin’	0.508	

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Correction method= # Reported T Limits: Tmin=0.560 Tmax=0.610
AbsCorr = MULTI-SCAN

Data completeness= 0.903          Theta(max)= 28.843

R(reflections)= 0.0309( 4642)     wR2(reflections)= 0.0945( 5715)

S = 1.017                 Npar= 296
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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

PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --C3 . 5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for O7 --C17 . 5.3 s.u.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C14 -C14_a 1.36 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H15 ..H20A 2.13 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H15 ..H20C 2.11 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Er1 --O7 . 6.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20C Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 3.50 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 109.9 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 111.4 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 366 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 4 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 14 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 2 Units

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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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
13 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 30/01/2018; check.def file version of 30/01/2018

Datablock 30_sq - ellipsoid plot