checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:  C-C = 0.0098 A          Wavelength=0.71073

Cell:            a=12.311(1)     b=19.775(2)         c=14.228(2)
                 alpha=90        beta=97.297(4)      gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	3435.8(7)	3435.8(7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H43 Cl N4 O Zr [+ solvent]	C28 H43 Cl N4 O Zr
Sum formula	C28 H43 Cl N4 O Zr [+ solvent]	C28 H43 Cl N4 O Zr
Mr	578.33	578.33
Dx,g cm-3	1.118	1.118
Z	4	4
Mu (mm-1)	0.420	0.420
F000	1216.0	1216.0
F000’	1204.93	
h,k,lmax	15,24,17	14,24,17
Nref	6526	6506
Tmin,Tmax	0.960,0.975	0.850,0.975
Tmin’	0.845	

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Correction method= # Reported T Limits: Tmin=0.850 Tmax=0.975
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.680

R(reflections)= 0.0657( 3182)     wR2(reflections)= 0.1808( 6506)

S = 0.878                 Npar= 310
```

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

PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

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Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 49% Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C28 . 3 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C26 . 3 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C27 . 3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00978 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 11.840 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.392 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H27C -0.33 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 404 A**3
PLAT793_ALERT_4_G Model has Chirality at N1 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at N3 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1 (IV) . 4.39 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 24 Note
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 !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.0 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

3 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
12 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
2 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 shelx - ellipsoid plot

