

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Zn-BpTzTz-Isopht

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: Zn-BpTzTz-Isopht

Bond precision: C-C = 0.0040 A

Wavelength=0.71073

Cell: a=9.1388(6) b=10.0354(7) c=14.2804(11)
 alpha=88.417(4) beta=88.236(5) gamma=75.636(4)
Temperature: 100 K

	Calculated	Reported
Volume	1267.86(16)	1267.86(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H12 N4 O4 S2 Zn, C3 H7 N O	C22 H12 N4 O4 S2 Zn, C3 H7 N O
Sum formula	C25 H19 N5 O5 S2 Zn	C25 H19 N5 O5 S2 Zn
Mr	598.96	598.94
Dx,g cm-3	1.569	1.569
Z	2	2
Mu (mm-1)	1.181	1.181
F000	612.0	612.0
F000'	613.28	
h,k,lmax	11,12,17	11,12,17
Nref	4888	4743
Tmin,Tmax	0.932,0.988	0.695,0.746
Tmin'	0.889	

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.970

Theta(max)= 25.799

R(reflections)= 0.0400(3696)

wR2(reflections)= 0.0916(4743)

S = 1.055

Npar= 364

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.970	Why?
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	2	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C23	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	135	Report



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn --O4_d .	6.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn --C8_d .	5.9	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	12%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	40%	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11	Ratio
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	9	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	5	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
4 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 09/11/2017; check.def file version of 08/11/2017

