

Datablock: 3

Bond precision: C-C = 0.0062 A Wavelength=0.71073
Cell: a=13.0826(10) b=10.2506(7) c=13.1685(13)
alpha=90 beta=111.237(10) gamma=90
Temperature 293 K
:
Calculated Reported
Volume 1646.0(3) 1646.0(3)
Space group P 21/c P 21/c
Hall group -P 2ybc -P 2ybc
Moiety formula C10 H16 N10 O S Zn ?
Sum formula C10 H16 N10 O S Zn C10 H16 N10 O S Zn
Mr 389.78 389.76
Dx, g cm-3 1.573 1.573
Z 4 4
Mu (mm-1) 1.639 1.639
F000 800.0 800.0
F000' 801.77
h, k, lmax 16, 13, 17 16, 13, 17
Nref 3780 3779
Tmin, Tmax 0.560, 0.721 0.546, 1.000
Tmin' 0.370
Correction method= # Reported T Limits: Tmin=0.546
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 1.000 Theta(max)= 27.479
R(reflections)= 0.0481(2489) wR2(reflections)=
0.1230(3779)
S = 1.084 Npar= 212

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

[PLAT230_ALERT_2_B](#) Hirshfeld Test Diff for N8 --N9 . 25.7 s.u.

**Author Response: The anomalous data for Hirshfeld test is an artefact in the structure.
According to other characterizations there is no doubt that azide ligand, three connected N atoms, is coordinated to Zn.**

[PLAT230_ALERT_2_B](#) Hirshfeld Test Diff for N9 --N10 . 24.4 s.u.

**Author Response: The anomalous data for Hirshfeld test is an artefact in the structure.
According to other characterizations there is no doubt that azide ligand, three connected N atoms, is coordinated to Zn.**

[PLAT242_ALERT_2_B](#) Low 'MainMol' Ueq as Compared to Neighbors of N9 Check

Author Response: The azide ligand is terminal group, false alarm occurs.

●Alert level C

[PLAT220_ALERT_2_C](#) NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.1 Ratio

[PLAT241_ALERT_2_C](#) High 'MainMol' Ueq as Compared to Neighbors of N8 Check

[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of N6 Check

Author Response: The azide ligand is terminal group, false alarm occurs.

[PLAT341_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00625 Ang.

[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 2.586 Check

●Alert level G

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 --N2 .	5.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 --N8 .	5.7	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.95	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
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low
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
3 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
0 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

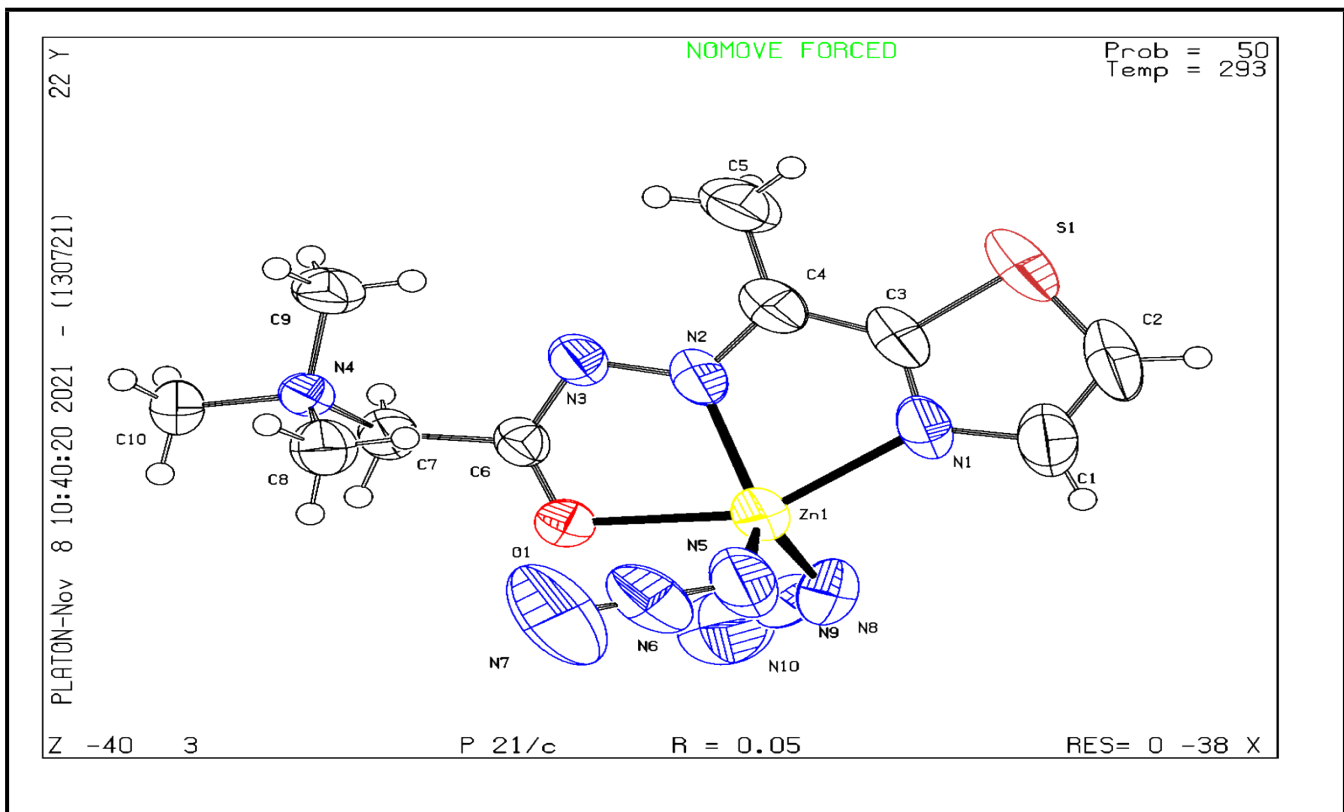
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/07/2021; check.def file version of 13/07/2021

Datablock 3 - ellipsoid plot



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