

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ZnL1

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: ZnL1

Bond precision: C-C = 0.0043 Å Wavelength=0.71073

Cell: a=12.5192(9) b=24.7373(18) c=11.2498(8)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

| | Calculated | Reported |
|----------------|------------------|------------------|
| Volume | 3484.0(4) | 3484.0(4) |
| Space group | P n m a | P n m a |
| Hall group | -P 2ac 2n | -P 2ac 2n |
| Moiety formula | C46 H32 N2 O4 Zn | C46 H32 N2 O4 Zn |
| Sum formula | C46 H32 N2 O4 Zn | C46 H32 N2 O4 Zn |
| Mr | 742.13 | 742.10 |
| Dx,g cm-3 | 1.415 | 1.415 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.755 | 0.755 |
| F000 | 1536.0 | 1536.0 |
| F000' | 1537.71 | |
| h,k,lmax | 15,30,14 | 15,30,14 |
| Nref | 3648 | 3646 |
| Tmin,Tmax | 0.897,0.963 | 0.929,1.000 |
| Tmin' | 0.712 | |

Correction method= # Reported T Limits: Tmin=0.929 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.389

R(reflections)= 0.0517(2709) wR2(reflections)= 0.1629(3646)

S = 1.022 Npar= 300

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

| | | | |
|-------------------|--|-----|-------|
| PLAT162_ALERT_4_C | Missing or Zero s.u. (esd) on y-coordinate for . | 05 | Check |
| PLAT162_ALERT_4_C | Missing or Zero s.u. (esd) on y-coordinate for . | 06 | Check |
| PLAT162_ALERT_4_C | Missing or Zero s.u. (esd) on y-coordinate for . | C26 | Check |
| PLAT162_ALERT_4_C | Missing or Zero s.u. (esd) on y-coordinate for . | C27 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | Zn1 | Check |

● Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C46 H32 N2 O4 Zn1
Atom count from the _atom_site data: C45.84400 H31.92199 N2 O3.844 Zn
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C46 H32 N2 O4 Zn
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|------|
| C | 184.00 | 183.38 | 0.62 |
| H | 128.00 | 127.69 | 0.31 |
| N | 8.00 | 8.00 | 0.00 |
| O | 16.00 | 15.38 | 0.62 |
| Zn | 4.00 | 4.00 | 0.00 |

| | | | |
|-------------------|--|------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 13 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 8 | Report |
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large | 0.10 | Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records | 7 | Report |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU 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 |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H23A Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H23B Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H23C Constrained at | 0.5 | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 8% | Note |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C22 - C23 . | 1.55 | Ang. |
| PLAT789_ALERT_4_G | Atoms with Negative _atom_site_disorder_group # | 14 | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 123 | Note |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 1 | Note |

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
18 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

