checkCIF/PLATON report

Structure factors have been supplied for datablock(s) oc-5

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: oc-5**

**Bond precision:** C-C = 0.0045 Å

**Cell:**
- \(a = 8.708(3)\)
- \(b = 11.863(5)\)
- \(c = 13.528(5)\)
- \(\alpha = 87.872(19)\)
- \(\beta = 77.546(19)\)
- \(\gamma = 83.842(19)\)

**Temperature:** 299 K

**Volume**
- Calculated: 1356.6(9)
- Reported: 1356.6(9)

**Space group:** P -1

**Hall group:** -P 1 -P 1

**Moiety formula:** 2(C28 H40 N4 O2), 0.5(H2 O)

**Sum formula:** C56 H81 N8 O4.50

**Mr:** 938.29

**Dx, g cm\(^{-3}\):**
- Calculated: 1.148
- Reported: 1.149

**Z:**
- Calculated: 1
- Reported: 2

**Mu (mm\(^{-1}\):**
- Calculated: 0.368
- Reported: 0.368

**F000:**
- Calculated: 509.0
- Reported: 509.0

**F000’:**
- Calculated: 510.04

**h,k,lmax:**
- Calculated: 10,14,16
- Reported: 10,14,16

**Nref:**
- Calculated: 4823
- Reported: 4807

**Tmin, Tmax:**
- Calculated: 0.957, 0.964
- Reported: 0.482, 0.751

**Tmin’:**
- Calculated: 0.929

**Correction method:** # Reported T Limits: Tmin=0.482 Tmax=0.751

AbsCorr = MULTI-SCAN

**Data completeness:** 0.997

**Theta(max):** 53.158

**R(reflections):** 0.0725 (2930)

**wR2(reflections):** 0.2243 (4807)

**S:** 1.050

**Npar:** 321
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**

- **PLAT042_ALERT_1_C** Calc. and Reported MoietyFormula Strings Differ Please Check
- **PLAT241_ALERT_4_C** Unitcell Contains Non-integer Number of Atoms Please Check
- **PLAT242_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C26 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of N2 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of C14 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of C16 Check
- **PLAT260_ALERT_2_C** Large Average Ueq of Residue Including O4 0.160 Check
- **PLAT340_ALERT_3_C** Low Bond Precision on C-C Bonds 0.00452 Ang.
- **PLAT414_ALERT_2_C** Short Intra D-H..H-X H4 ..H14 1.93 Ang. x,y,z = 1_555 Check
- **PLAT911_ALERT_3_C** Missing FCF Refl Between Thmin & STh/L= 0.597 17 Report

---

**Alert level G**

- **ABSMU01_ALERT_1_G** Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.
- **PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite 3 Note
- **PLAT007_ALERT_5_G** Number of Unrefined Donor-H Atoms 3 Report
- **PLAT045_ALERT_1_G** Calculated and Reported Z Differ by a Factor ... 0.500 Check
- **PLAT072_ALERT_2_G** SHELXL First Parameter in WGHT Unusually Large 0.13 Report
- **PLAT154_ALERT_1_G** The s.u.’s on the Cell Angles are Equal ..(Note) 0.019 Degree
- **PLAT172_ALERT_4_G** The CIF-Embedded .res File Contains DFIX Records 2 Report
- **PLAT300_ALERT_4_G** Atom Site Occupancy of O4 Constrained at 0.25 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H4A Constrained at 0.25 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H4B Constrained at 0.25 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 ) 0.75 Check
- **PLAT415_ALERT_2_G** Short Inter D-H..H-X H11B ..H4A 2.13 Ang. x,y,z = 1_555 Check
- **PLAT415_ALERT_2_G** Short Inter D-H..H-X H11B ..H4B 2.08 Ang. 2-x,1-y,-z = 2_765 Check
- **PLAT789_ALERT_4_G** Atoms with Negative _atom_site_disorder_group # 3 Check
- **PLAT793_ALERT_4_G** Model has Chirality at C6 (Centro SPGR) S Verify
- **PLAT860_ALERT_3_G** Number of Least-Squares Restraints ............... 2 Note
- **PLAT883_ALERT_1_G** No Info/Value for _atom_sites_solution_primary Please Do !
- **PLAT978_ALERT_2_G** Number C-C Bonds with Positive Residual Density. 0 Info
- **PLAT992_ALERT_5_G** Repd & Actual _reflns_number_gt Values Differ by 3 Check

---

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

5 **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
3 **ALERT type 3** Indicator that the structure quality may be low
9 **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 18/05/2022; check.def file version of 17/05/2022**