

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 12_18srv479

Bond precision: C-C = 0.0092 Å Wavelength=1.54178

Cell: a=19.5114 (12) b=9.7395 (6) c=19.9893 (12)
alpha=90 beta=107.714 (4) gamma=90

Temperature: 120 K

| | Calculated | Reported |
|----------------|--------------------|--------------------|
| Volume | 3618.5 (4) | 3618.5 (4) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C47 H32 O, C4 H8 O | C47 H32 O, C4 H8 O |
| Sum formula | C51 H40 O2 | C51 H40 O2 |
| Mr | 684.83 | 684.83 |
| Dx, g cm-3 | 1.257 | 1.257 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.577 | 0.577 |
| F000 | 1448.0 | 1448.0 |
| F000' | 1451.91 | |
| h, k, lmax | 23,11,23 | 23,11,23 |
| Nref | 6520 | 6478 |
| Tmin, Tmax | 0.966, 0.989 | 0.873, 1.000 |
| Tmin' | 0.955 | |

Correction method= # Reported T Limits: Tmin=0.873 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta (max)= 67.494

R(reflections)= 0.1092 (2662) wR2 (reflections)=
0.2929 (6478)
S = 0.987 Npar= 475

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 A**

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.311

Author Response: The high value of Rint is caused by extremely weak diffraction from the crystals in spite of collecting data using Cu-radiation and with a long exposure time.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.311 Report

Author Response: The high value of Rint is caused by extremely weak diffraction from the crystals in spite of collecting data using Cu-radiation and with a long exposure time.

 **Alert level B**

PLAT420_ALERT_2_B D-H Bond Without Acceptor O1 --H1 . Please Check

 **Alert level C**

| | |
|--|--------------|
| PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. | 41% Check |
| PLAT082_ALERT_2_C High R1 Value | 0.11 Report |
| PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) | 0.29 Report |
| PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds | 0.00918 Ang. |

 **Alert level G**

| | |
|--|--------------|
| PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite | 9 Note |
| PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms | 1 Report |
| PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF | Please Check |
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large | 0.12 Report |
| PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records | 3 Report |
| PLAT300_ALERT_4_G Atom Site Occupancy of C1SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C1SB Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C2SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C2SB Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C3SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C3SB Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C4SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C4SB Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H1SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H1SB Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H1SC Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H1SD Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H2SA Constrained at | 0.5 Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H2SB Constrained at | 0.5 Check |

| | | | | |
|-------------------|--|----------------|-------|--------|
| PLAT300_ALERT_4_G | Atom Site Occupancy of H2SC | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H2SD | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3SA | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3SB | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3SC | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3SD | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4SA | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4SB | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4SC | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4SD | Constrained at | 0.5 | Check |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 2) | | 80% | Note |
| PLAT398_ALERT_2_G | Deviating C-O-C Angle From 120 for O2 | | 11.8 | Degree |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | 24 | Note |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | | 13 | Note |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | | 1 | Note |
| PLAT967_ALERT_5_G | Note: Two-Theta Cutoff Value in Embedded .res .. | | 135.0 | Degree |

2 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

27 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 18/12/2021; check.def file version of 18/12/2021

Datablock 12_18srv479 - ellipsoid plot

