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: I

Bond precision: C-C = 0.0451 A Wavelength=0.71073

Cell: a=12.6390(15) b=12.6459(14) c=15.8527(18)
alpha=78.916(3) beta=75.930(3) gamma=71.011(1)
Temperature: 298 K

	Calculated	Reported
Volume	2306.3(5)	2306.3(5)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C78 H70 Er2 N4 O12, 4(C2 H6 O)	?
Sum formula	C86 H94 Er2 N4 O16	C86 H94 Er2 N4 O16
Mr	1774.17	1774.17
Dx,g cm-3	1.277	1.277
Z	1	1
Mu (mm-1)	1.866	1.866
F000	902.0	902.0
F000’	901.84	
h,k,lmax	15,15,18	15,15,18
Nref	8130	7848
Tmin,Tmax	0.735,0.878	0.742,0.880
Tmin’	0.721	

Correction method= # Reported T Limits: Tmin=0.742 Tmax=0.880
AbsCorr = MULTI-SCAN

Data completeness= 0.965 Theta(max)= 25.020

R(reflections)= 0.1444(4959) wR2(reflections)= 0.3470(7848)

S = 1.090 Npar= 488

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Er1 --O4_a . 10.1 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference C34 --C35 . 0.30 Ang.
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.04512 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C1 - C2 . 1.57 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C10 - C11 . 1.59 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C31 - C38 . 1.59 Ang.
PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 171 Ang**3

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.124
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.124 Report
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.965 Why?
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ..... Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.14 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.35 Report
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... Please Do !
PLAT213_ALERT_2_C Atom C26 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C33 has ADP max/min Ratio ..... 3.3 oblate
PLAT213_ALERT_2_C Atom C38 has ADP max/min Ratio ..... 3.7 oblate
PLAT234_ALERT_4_C Large Hirshfeld Difference Er1 --O6 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C1 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12 --C13 . 0.24 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Er1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C40 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O7 0.229 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O8 0.160 Check
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C15 - C16 . 1.54 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C30 - C31 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C33 - C34 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C34 - C39 . 1.53 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 16 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 21 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 72.49 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C2 -C7 . 1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C11 -C16 . 1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C31 -C38 . 1.50 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C11 -C16 0.16 Ang.

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PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C31      -C38            0.30 Ang.
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C9       -H9C            1.555   1.555 ........     #   42 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C17      -H17A           1.555   1.555 ........     #   55 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97000 Dev...       0.01 Ang.
             C40      -H40B           1.555   1.555 ........     #  101 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97000 Dev...       0.01 Ang.
             C42      -H42B           1.555   1.555 ........     #  107 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        251 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/       2018 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
  30 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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  33 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author’s name and address are missing,
            _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. ’Acta Crystallographica Section C’
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

```
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock I - ellipsoid plot