



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) oner114-OMe-3-CH3

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: oner114-OMe-3-CH3

Bond precision:	C-C = 0.0034 Å	Wavelength=0.71073
Cell:	a=12.3499(18) alpha=90	b=6.6311(9) beta=95.129(4) c=18.640(3) gamma=90
Temperature:	273 K	
	Calculated	Reported
Volume	1520.4(4)	1520.4(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C17 H12 F3 N O	C17 H12 F3 N O
Sum formula	C17 H12 F3 N O	C17 H12 F3 N O
Mr	303.28	303.29
Dx, g cm ⁻³	1.325	1.325
Z	4	4
Mu (mm ⁻¹)	0.108	0.108
F000	624.0	624.5
F000'	624.41	
h, k, lmax	15, 8, 23	15, 8, 23
Nref	3133	3122
Tmin, Tmax	0.988, 0.991	0.564, 0.745
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.564 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 26.410

R(reflections)= 0.0524(1476)

wR2(reflections)=
0.1524(3122)

S = 1.028

Npar= 228

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	47% Check
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C8 --C10 .	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C15 --C16 .	5.5 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F1 --C1 .	0.18 Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C14 Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-8.581 Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
	0 0 2, 0 0 4,	



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7 Note
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT073_ALERT_1_G	H-atoms ref., but hydrogen treatment Reported as	constr Check
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	273 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	273 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C1 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	14% Note
PLAT769_ALERT_4_G	CIF Embedded Explicitly Supplied Scattering Data	5 Note
PLAT795_ALERT_4_G	C-Atom in CIF Coordinate List Out-of-Sequence ..	C7 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6 Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.07 Note
	-1 0 1,	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	6 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
	-1 0 1,	
PLAT948_ALERT_5_G	Externally Supplied Scattering Factors CIF	5 Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.947 Note
	Predicted wR2: Based on SigI**2 3.86 or SHELX Weight 14.84	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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

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

8 **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

6 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
6 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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: ...
;
_vrf_ABSTY02_oner114-OMe-3-CH3
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT026_oner114-OMe-3-CH3
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low ..          47% Check
RESPONSE: ...
;
_vrf_PLAT230_oner114-OMe-3-CH3
;
PROBLEM: Hirshfeld Test Diff for      C8      --C10      .      7.0 s.u.
RESPONSE: ...
;
_vrf_PLAT234_oner114-OMe-3-CH3
;
```

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PROBLEM: Large Hirshfeld Difference Fl      --C1      .      0.18 Ang.
RESPONSE: ...
;
_vrf_PLAT242_oner114-OMe-3-CH3
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of      C14 Check
RESPONSE: ...
;
_vrf_PLAT905_oner114-OMe-3-CH3
;
PROBLEM: Negative K value in the Analysis of Variance ...      -8.581 Report
RESPONSE: ...
;
_vrf_PLAT911_oner114-OMe-3-CH3
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      2 Report
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 04/06/2025; check.def file version of 30/05/2025

duplicate check

No duplication found

