

checkCIF (full publication check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

[Structure factor report](#)

Datablock: I

Bond precision:	C-C = 0.0032 Å	Wavelength=0.71073
Cell:	a=6.1702(13) b=7.1689(15) c=15.438(3)	
	alpha=90 beta=99.423(4) gamma=90	
Temperature: 150 K		
	Calculated	Reported
Volume	673.7(2)	673.7(2)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C14 H16 N4	C14 H16 N4
Sum formula	C14 H16 N4	C14 H16 N4
Mr	240.31	240.31
Dx, g cm ⁻³	1.185	1.185
Z	2	2
Mu (mm ⁻¹)	0.074	0.074
F000	256.0	256.0
F000'	256.07	
h,k,lmax	7,8,18	7,8,18
Nref	2476[1346]	2283
Tmin,Tmax	0.983,0.993	0.573,0.745
Tmin'	0.980	
Correction method=	# Reported T Limits: Tmin=0.573 Tmax=0.745	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.70/0.92	Theta(max)= 25.340
R(reflections)=	0.0363(2180)	wR2(reflections)= 0.0948(2283)
S =	1.109	Npar= 163

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

[STRVA01_ALERT_4_C](#) Flack test results are meaningless.

From the CIF: _refine_ls_abs_structure_Flack 0.100

From the CIF: _refine_ls_abs_structure_Flack_su 1.000

[PLAT910_ALERT_3_C](#) Missing # of FCF Reflection(s) Below Theta(Min).

5 Note

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600

7 Report

[PLAT915_ALERT_3_C](#) No Flack x Check Done: Low Friedel Pair Coverage

84 %

🟢 Alert level G

[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms

2 Report

[PLAT032_ALERT_4_G](#) Std. Uncertainty on Flack Parameter Value High .

1.000 Report

PLAT300_ALERT_4_G Atom Site Occupancy of H3A Constrained at 0.5 Check

And 5 other PLAT300 Alerts

More ...

PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C2 - C3 . 1.50 Ang.

PLAT791_ALERT_4_G Model has Chirality at C1 (Chiral SPGR) S Verify

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

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

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

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

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

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

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

9 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

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.

PUBL012_ALERT_1_A _publ_section_abstract is missing.

Abstract of paper in English.

PUBL024_ALERT_1_A The number of authors is greater than 9.

Please specify the role of each of the co-authors
for your paper.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

4 **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_PUBL006_GLOBAL

;

PROBLEM: _publ_requested_journal is missing

RESPONSE: ...

;

_vrf_PUBL008_GLOBAL

;

PROBLEM: _publ_section_title is missing. Title of paper.

RESPONSE: ...

;

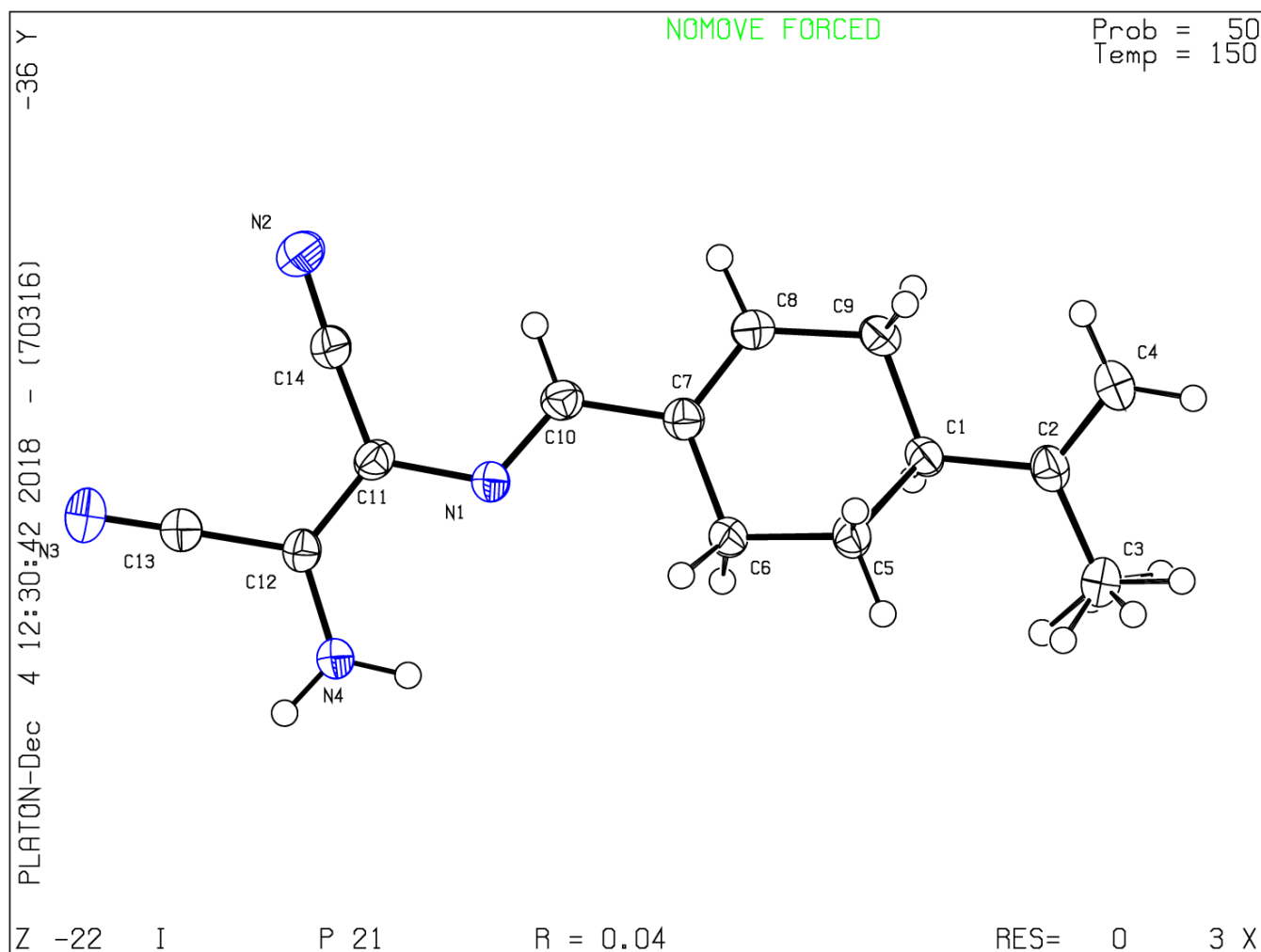
_vrf_PUBL012_GLOBAL

```
;  
PROBLEM: _publ_section_abstract is missing.  
RESPONSE: ...  
;  
_vrf_PUBL024_GLOBAL  
;  
PROBLEM: The number of authors is greater than 9.  
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 19/10/2018; check.def file version of 15/10/2018

Datablock I - ellipsoid plot



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