

## 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 = 0.0061 Å	Wavelength=0.71073
Cell:	a=11.6743(15)    b=14.0675(18)    c=25.660(4)	
	alpha=90    beta=94.342(3)    gamma=90	
Temperature: 150 K		
	Calculated	Reported
Volume	4202.0(10)	4202.1(10)
Space group	I 2	I 2
Hall group	I 2y	I 2y
Moiety formula	C24 H30 N2 O	C48 H60 N4 O2
Sum formula	C24 H30 N2 O	C48 H60 N4 O2
Mr	362.50	725.00
Dx, g cm <sup>-3</sup>	1.146	1.146
Z	8	4
Mu (mm <sup>-1</sup> )	0.070	0.070
F000	1568.0	1568.0
F000'	1568.56	
h,k,lmax	14,16,30	14,16,30
Nref	7694[ 4019]	7592
Tmin,Tmax	0.982,0.994	0.654,0.745
Tmin'	0.982	
Correction method=	# Reported T Limits: Tmin=0.654 Tmax=0.745	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.89/0.99	Theta(max)= 25.343
R(reflections)=	0.0525( 6365)	wR2(reflections)= 0.1208( 7592)
S =	1.124	Npar= 504

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

PLAT201\_ALERT\_2\_B Isotropic non-H Atoms in Main Residue(s) ..... 2 Report

**Author Response: This alert arises due to the isotropic treatment used to model the disordered terminal methyl groups belonging to both individual molecules composing the asymmetric unit of the compound.**

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 16 Note

### Alert level C

STRVA01\_ALERT\_2\_C Chirality of atom sites is inverted?

From the CIF: `_refine_ls_abs_structure_Flack` 1.700

From the CIF: `_refine_ls_abs_structure_Flack_su` 0.900

PLAT220\_ALERT\_2\_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio  
PLAT220\_ALERT\_2\_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.9 Ratio  
PLAT222\_ALERT\_3\_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00613 Ang.  
PLAT907\_ALERT\_2\_C Flack x > 0.5, Structure Needs to be Inverted? . 1.70 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

## Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 8 Note  
PLAT032\_ALERT\_4\_G Std. Uncertainty on Flack Parameter Value High . 0.900 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 2.00 Check  
PLAT111\_ALERT\_2\_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 96 %Fit  
PLAT112\_ALERT\_2\_G ADDSYM Detects New (Pseudo) Symm. Elem c 88 %Fit  
PLAT113\_ALERT\_2\_G ADDSYM Suggests Possible Pseudo/New Space Group I2/c Check  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C48 Constrained at 0.6 Check

### And 15 other PLAT300 Alerts

More ...

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 4% Note  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 2 ) 4% Note  
PLAT791\_ALERT\_4\_G Model has Chirality at C15 (Chiral SPGR) S Verify

### And 3 other PLAT791 Alerts

More ...

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 5 Note  
PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter Values Differ by . 0.11 Check  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 12 Info

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

- 2 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  
7 ALERT type 3 Indicator that the structure quality may be low  
22 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

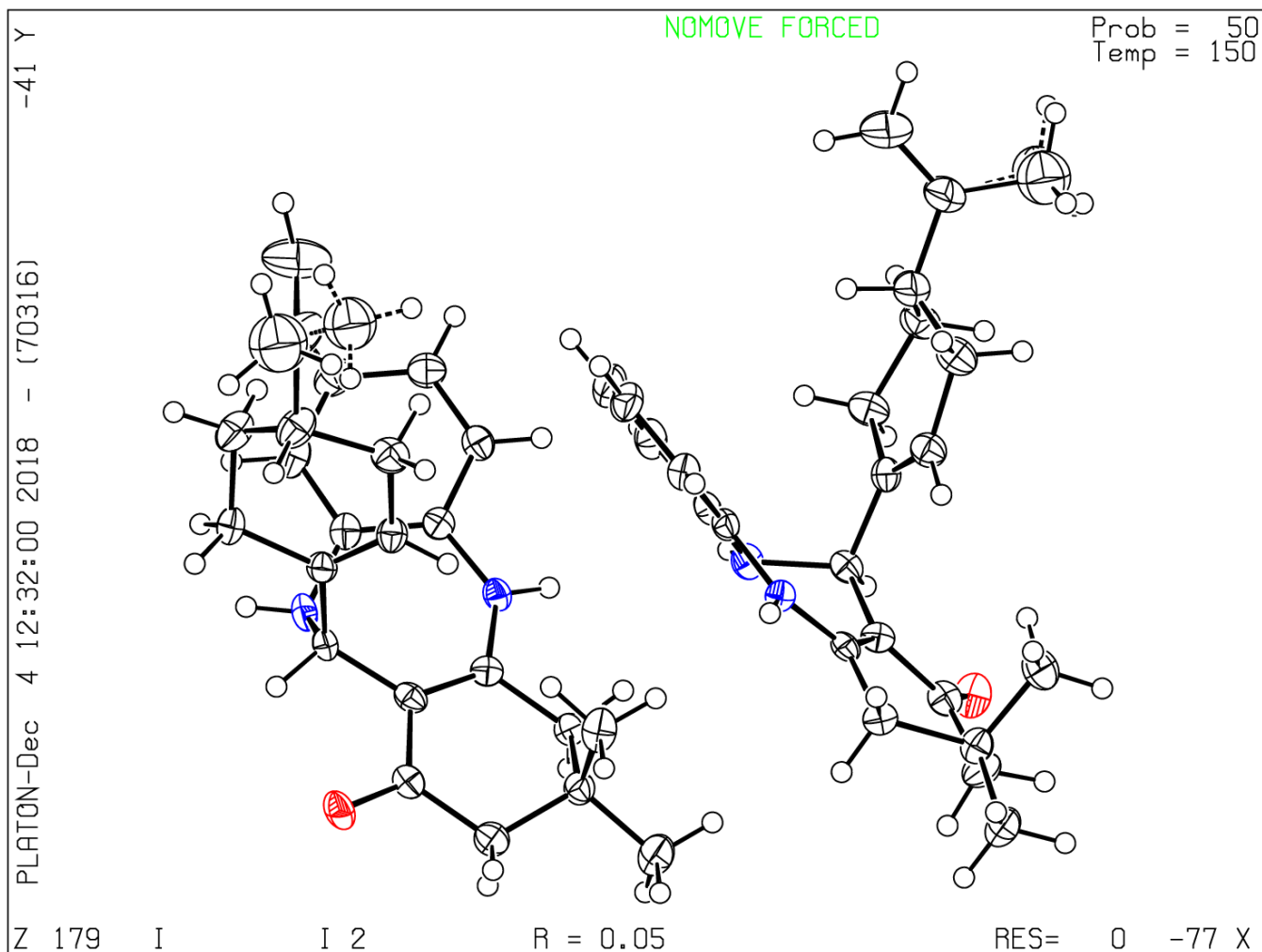
```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PUBL024_GLOBAL
;
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.

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PLATON version of 19/10/2018; check.def file version of 15/10/2018

## Datablock I - ellipsoid plot



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