

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

[report](#)

[Structure factor report](#)

[CIF dictionary](#)

[Interpreting this](#)

Datablock: 21104ocb

Bond precision: C-C = 0.0024 Å Wavelength=1.54184

Cell: a=12.2754(2) b=11.0203(2) c=22.3353(5)

alpha=90 beta=96.455(2) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	3002.33(10)	3002.33(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C35 H30 N2 O5 S	C35 H30 N2 O5 S
Sum formula	C35 H30 N2 O5 S	C35 H30 N2 O5 S
Mr	590.67	590.67
Dx, g cm ⁻³	1.307	1.307
Z	4	4
Mu (mm ⁻¹)	1.333	1.333
F000	1240.0	1240.0
F000'	1244.93	
h, k, lmax	14, 12, 25	14, 12, 25
Nref	4807	4777
Tmin, Tmax	0.739, 0.864	0.304, 1.000
Tmin'	0.605	

Correction method= # Reported T Limits: Tmin=0.304

Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 62.722

R(reflections)= 0.0374(4342) wR2(reflections)= 0.0946(4777)

S = 1.028 Npar= 389

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

[THETM01 ALERT 3 C](#) The value of $\sin(\theta_{\max})/\lambda$ is less than 0.590

Calculated $\sin(\theta_{\max})/\lambda = 0.5764$

[PLAT023 ALERT 3 C](#) Resolution (too) Low [$\sin(\theta)/\lambda < 0.6$].. 0.58 Ang-1

[PLAT420 ALERT 2 C](#) D-H Bond Without Acceptor N2 --H2A .
Please Check

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.576
30 Report

Alert level G

[PLAT007 ALERT 5 G](#) Number of Unrefined Donor-H Atoms
2 Report

[PLAT432 ALERT 2 G](#) Short Inter X...Y Contact O1 ..C45
3.00 Ang.

1-x,1-y,-z = 3_665

Check

[PLAT484 ALERT 4 G](#) Round D-H..A Angle Rep for N1 ..02 .
155 Degree

[PLAT484 ALERT 4 G](#) Round D-H..A Angle Rep for C45 ..01 .
111 Degree

[PLAT793 ALERT 4 G](#) Model has Chirality at C2 (Centro SPGR)
R Verify

And 2 other PLAT793 Alerts

More ...

[PLAT795 ALERT 4 G](#) C-Atom in CIF Coordinate List Out-of-Sequence ..
C2 Note

[PLAT796 ALERT 4 G](#) O-Atom in CIF Coordinate List Out-of-Sequence ..
O2 Note

[PLAT883 ALERT 1 G](#) No Info/Value for _atom_sites_solution_primary .
Please Do !

[PLAT909 ALERT 3 G](#) Percentage of I>2sig(I) Data at Theta(Max) Still
86% Note

[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity
2.9 Low

[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density.
8 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
13 **ALERT level G** = General information/check it is not something unexpected

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

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

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

7 ALERT type 4 Improvement, methodology, query or suggestion

1 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.

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.

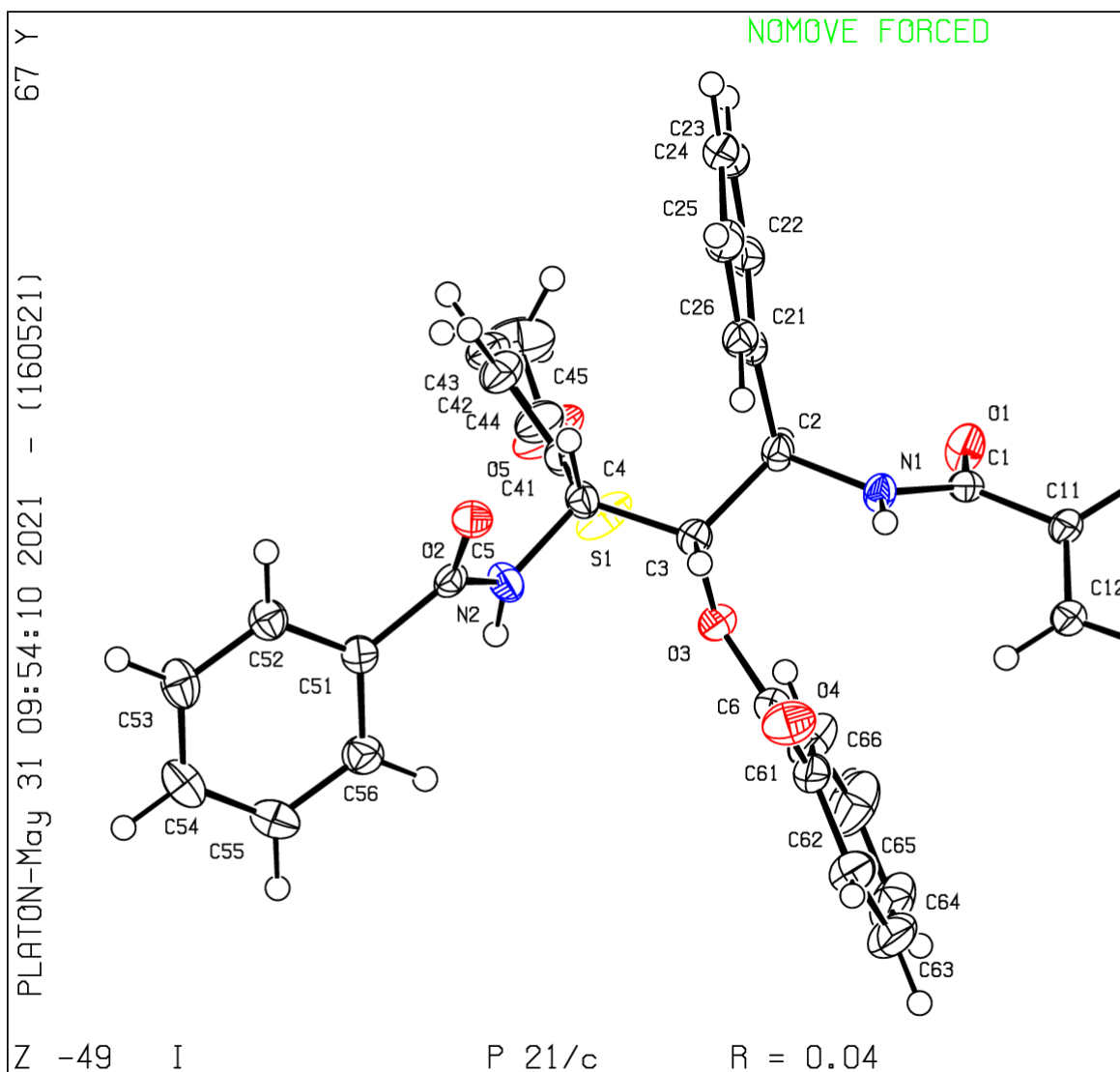
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
```

```
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 16/05/2021; check.def file version of 13/05/2021

Datablock I - ellipsoid plot



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