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. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: 21147ocl_sq

Bond precision: C-C = 0.0033 A Wavelength=1.54184
Cell: a=10.2985(3) b=26.7638(6) c=12.0788(4)
alpha=90 beta=111.086(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3106.32(18)	3106.32(17)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C35 H30 N2 O5 [+ solvent]	C35 H30 N2 O5 [+ solvent]
Sum formula	C35 H30 N2 O5 [+ solvent]	C35 H30 N2 O5
Mr	558.61	558.61
Dx,g cm-3	1.194	1.194
Z	4	4
Mu (mm-1)	0.648	0.648
F000	1176.0	1176.0
F000'	1179.60	
h,k,lmax	11,30,13	11,30,13
Nref	4974	4961
Tmin,Tmax	0.849,0.949	0.571,1.000
Tmin'	0.762	

Correction method= # Reported T Limits: Tmin=0.571 Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.997 Theta(max)= 62.723
R(reflections)= 0.0472(4348) wR2(reflections)= 0.1286(4961)
S = 1.038 Npar= 436

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5765
PLAT023_ALERT_3_C Resolution (too) Low [sin(theta)/Lambda < 0.6].. 0.58 Ang-1
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.88 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.71 eA-3
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.253 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.576 14 Report

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 6 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 14% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5 106.5 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 136 A**3
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SPGR) R Verify
And 2 other PLAT793 Alerts
More ...
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 75 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
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 57% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

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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

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

   2 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
   8 ALERT type 3 Indicator that the structure quality may be low
   8 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

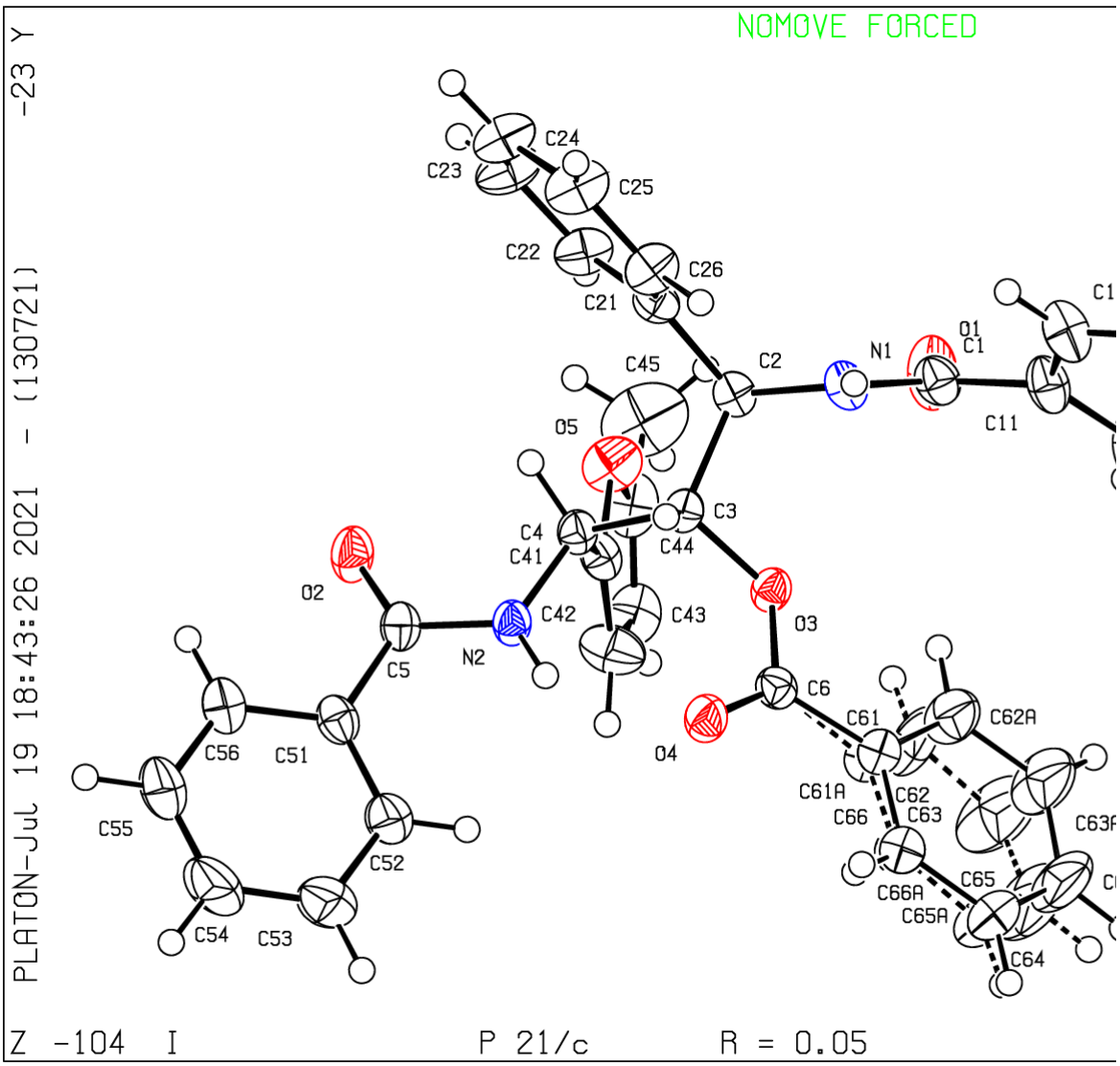
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# 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 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot



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Test a new CIF entry