checkCIF () running

Checking for embedded fcf data in CIF ...
No extractable fcf data in found in CIF

checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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.You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: C-C = 0.0021 A Wavelength=0.71073
Cell: a=29.831(2) b=29.831(2) c=9.7983(8)
alpha=90 beta=90 gamma=120
Temperature: 90 K

	Calculated	Reported
Volume	7551.2(14)	7551.2(11)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C17 H18 Cl N O5	C17 H18 Cl N O5
Sum formula	C17 H18 Cl N O5	C17 H18 Cl N O5
Mr	351.77	351.77
Dx,g cm-3	1.392	1.392
Z	18	18
Mu (mm-1)	0.254	0.254
F000	3312.0	3312.0
F000'	3316.34	
h,k,lmax	35,35,11	35,35,11
Nref	2975	2975
Tmin,Tmax	0.881,0.892	0.746,0.892
Tmin'	0.881	

Correction method= # Reported T Limits: Tmin=0.746 Tmax=0.892 AbsCorr = EMPIRICAL
Data completeness= 1.000 Theta(max)= 25.030
R(reflections)= 0.0270(2742) wR2(reflections)= 0.0943(2975)
S = 1.121 Npar= 221

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

PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 34 Ang3

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	6.67	Why ?
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	3	Units
PLAT793_ALERT_4_G	The Model has Chirality at C10 (Centro SPGR)	R	Verify

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

1 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
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

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).

2 **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.

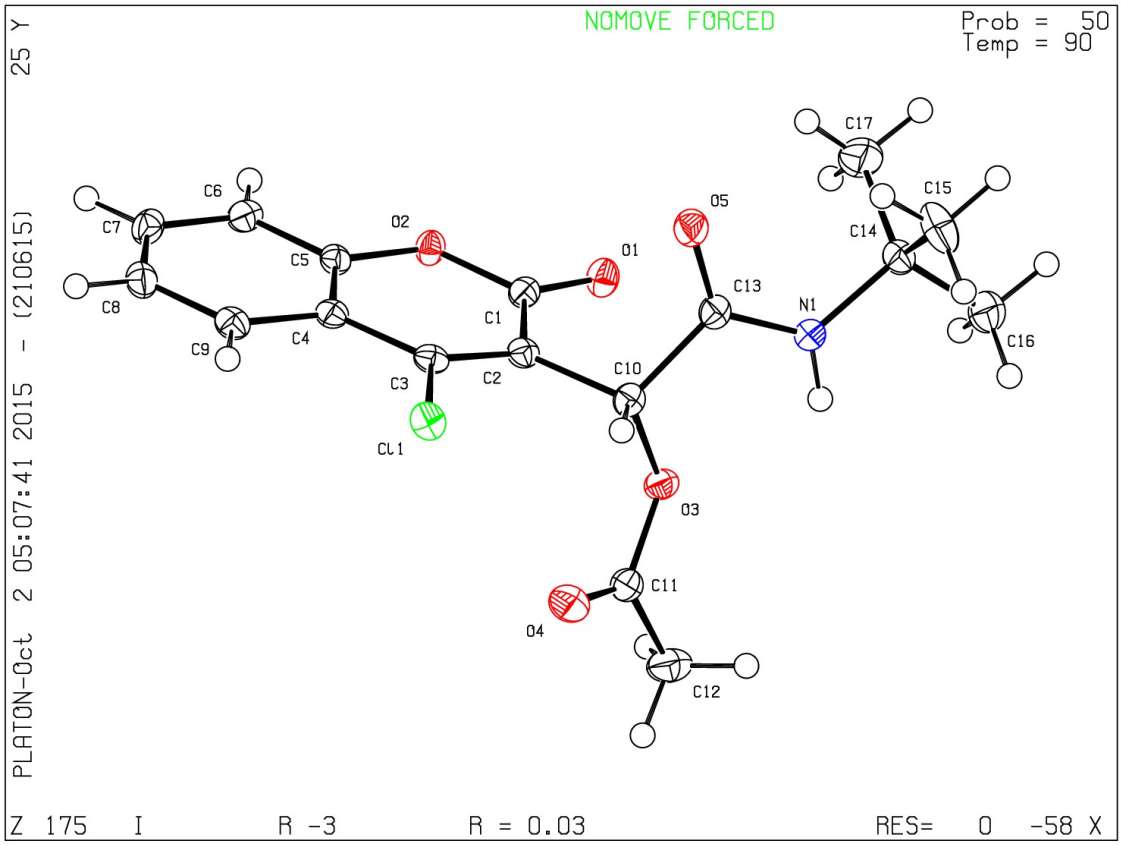
Validation response form
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_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: ...
;
# 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 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 21/06/2015; check.def file version of 21/06/2015

Datablock I – ellipsoid plot



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Test a new CIF entry