

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 = 0.0012 Å Wavelength=0.71073
 Cell: a=9.3350 (5) b=4.8453 (2) c=13.1633 (6)
 alpha=90 beta=105.1101 (14) gamma=90
 Temperature: 100 K

	Calculated	Reported
Volume	574.80 (5)	574.80 (5)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C6 H15 N4 O2, H2 O3 P	C6 H15 N4 O2, H2 O3 P
Sum formula	C6 H17 N4 O5 P	C6 H17 N4 O5 P
Mr	256.21	256.20
Dx, g cm ⁻³	1.480	1.480
Z	2	2
Mu (mm ⁻¹)	0.254	0.254
F000	272.0	272.0
F000'	272.34	
h, k, lmax	15, 8, 21	15, 8, 21
Nref	5594 [3056]	5406
Tmin, Tmax	0.899, 0.924	0.710, 0.747
Tmin'	0.899	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.747
 AbsCorr = MULTI-SCAN
 Data completeness= 1.77/0.97 Theta(max)= 36.351
 R(reflections)= 0.0208 (5290) wR2(reflections)= 0.0534 (5406)
 S = 1.119 Npar= 176

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

[PLAT480_ALERT_4_C](#) Long H...A H-Bond Reported H3C .. O3 .. 2.64 Ang.
[PLAT480_ALERT_4_C](#) Long H...A H-Bond Reported H1 .. O3 .. 2.65 Ang.
[PLAT481_ALERT_4_C](#) Long D...A H-Bond Reported P1 .. O3 .. 3.92 Ang.
[PLAT911_ALERT_3_C](#) Missing # FCF Refl Between THmin & STh/L= 0.600 8 Report

● Alert level G

[PLAT791_ALERT_4_G](#) The Model has Chirality at C2 (Chiral SPGR) S Verify

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)	3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	14 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ...	3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	4 Note

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
 6 **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
 3 ALERT type 3 Indicator that the structure quality may be low
 5 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.

3 **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

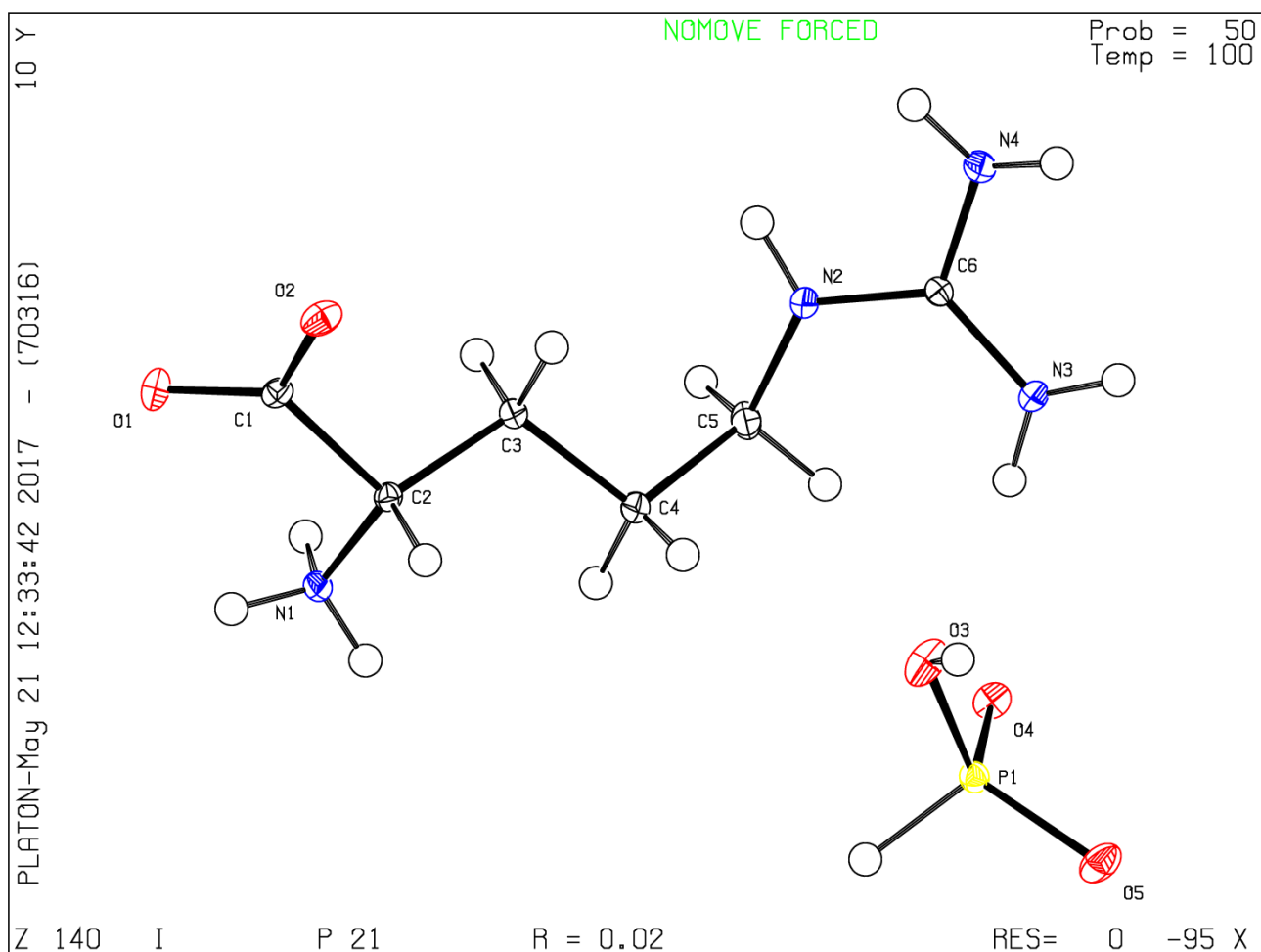
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_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: ...
;
# 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 27/03/2017; check.def file version of 24/03/2017

Datablock I - ellipsoid plot



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