

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 = 0.0105 Å	Wavelength=0.71075
Cell:	a=17.2782(6) b=17.5532(6) c=41.2439(12)	
	alpha=90 beta=90 gamma=90	
Temperature: 200 K		

	Calculated	Reported
Volume	12508.8(7)	12508.8(7)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C40 H24, 2(C16 H32 Li 04)	?
Sum formula	C72 H88 Li2 O8	C72 H88 Li2 O8
Mr	1095.30	1095.30
Dx, g cm-3	1.163	1.163
Z	8	8
Mu (mm-1)	0.073	0.073
F000	4720.0	4720.0
F000'	4722.03	
h,k,lmax	22,22,53	22,22,53
Nref	28695[15474]	28667
Tmin,Tmax	0.993,0.993	
Tmin'	0.993	

Correction method= Not given

Data completeness= 1.85/1.00 Theta(max)= 27.486

R(reflections)= 0.0742(11545) wR2(reflections)= 0.2044(28667)

S = 0.933 Npar= 1477

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

[PLAT241_ALERT_2_B](#) High 'MainMol' Ueq as Compared to Neighbors of C102 Check
[PLAT241_ALERT_2_B](#) High 'MainMol' Ueq as Compared to Neighbors of C110 Check
[PLAT242_ALERT_2_B](#) Low 'MainMol' Ueq as Compared to Neighbors of C101 Check
[PLAT340_ALERT_3_B](#) Low Bond Precision on C-C Bonds 0.01051 Ang.
[PLAT910_ALERT_3_B](#) Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

Alert level C

[RINTA01_ALERT_3_C](#) The value of Rint is greater than 0.12
 Rint given 0.146
[STRVA01_ALERT_2_C](#) Chirality of atom sites is inverted?
 From the CIF: _refine_ls_abs_structure_Flack 1.200
 From the CIF: _refine_ls_abs_structure_Flack_su 0.600
[PLAT020_ALERT_3_C](#) The Value of Rint is Greater Than 0.12 0.146 Report
[PLAT026_ALERT_3_C](#) Ratio Observed / Unique Reflections (too) Low .. 40% Check
[PLAT048_ALERT_1_C](#) MoietyFormula Not Given (or Incomplete) Please Check
[PLAT221_ALERT_2_C](#) Solv./Anion Resd 4 C Ueq(max)/Ueq(min) Range 4.3 Ratio
[PLAT223_ALERT_4_C](#) Solv./Anion Resd 4 H Ueq(max)/Ueq(min) Range 4.3 Ratio
[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for C109 --C110 . 5.1 s.u.
[PLAT234_ALERT_4_C](#) Large Hirshfeld Difference C75 --C76 . 0.16 Ang.

And 5 other PLAT234 Alerts

[More ...](#)

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C82 Check
And 14 other PLAT241 Alerts
 More ...

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O1 Check
And 14 other PLAT242 Alerts
 More ...

PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1 0.111 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O5 0.111 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C89 - C90 . 1.36 Ang.
And 10 other PLAT360 Alerts
 More ...

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 7.854 Check
And 2 other PLAT906 Alerts
 More ...

PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 1.20 Check

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.600 Report
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ! Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.10 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 53 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

7 **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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
```

```

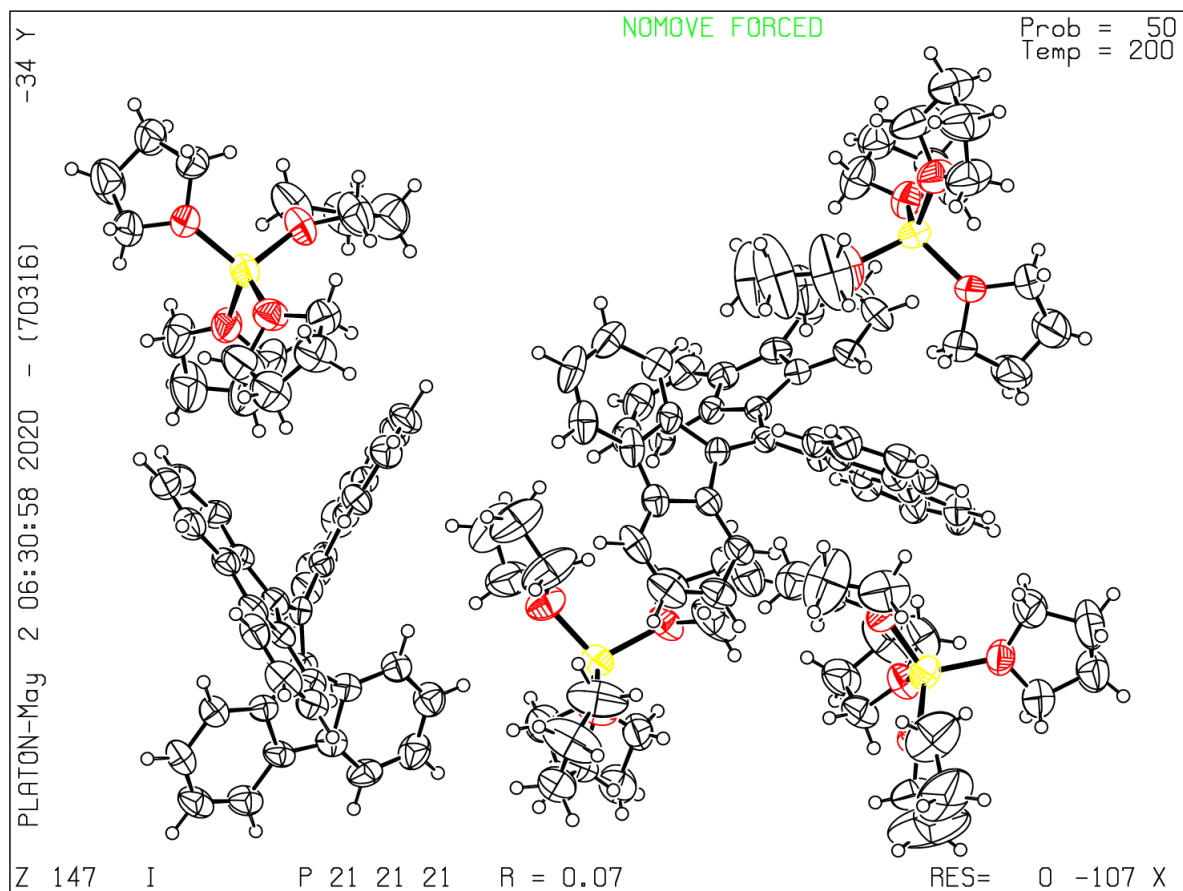
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
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 22/04/2020; check.def file version of 09/03/2020

Datablock I - ellipsoid plot



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