

# checkCIF/PLATON report

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.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: I

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Bond precision:    C-C = 0.0182 Å

Wavelength=1.34139

Cell:                a=15.3986(9)                b=15.4175(8)                c=17.9599(10)  
                      alpha=113.169(2)        beta=99.213(2)        gamma=103.219(2)  
Temperature:    173 K

	Calculated	Reported
Volume	3664.1(4)	3664.1(4)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C42 H70 O35, C10 H16 O [+ solvent]	C42 H70 O35, C10 H16 O [+ SOLVENT]
Sum formula	C52 H86 O36 [+ solvent]	C104 H172 O72
Mr	1287.21	2574.41
Dx, g cm <sup>-3</sup>	1.167	1.167
Z	2	1
Mu (mm <sup>-1</sup> )	0.545	0.545
F000	1372.0	1372.0
F000'	1376.09	
h,k,lmax	18,18,21	18,18,21
Nref	27880[ 13940]	26218
Tmin,Tmax	0.925,0.957	0.925,0.957
Tmin'	0.922	

Correction method= # Reported T Limits: Tmin=0.925 Tmax=0.957  
AbsCorr = MULTI-SCAN

Data completeness= 1.88/0.94                Theta(max)= 54.914

R(reflections)= 0.1024( 19199)                wR2(reflections)= 0.2941( 26218)

S = 1.027                                        Npar= 1568

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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.

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### ● Alert level B

PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	0.95 eA-3
PLAT234_ALERT_4_B	Large Hirshfeld Difference C89 --C90	0.26 Ang.
PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds .....	0.01819 Ang.
PLAT415_ALERT_2_B	Short Inter D-H..H-X H9 ..H30A	1.96 Ang.
	1+x,y,z =	1_655 Check
PLAT415_ALERT_2_B	Short Inter D-H..H-X H18A ..H34	1.98 Ang.
	x,-1+y,z =	1_545 Check
PLAT415_ALERT_2_B	Short Inter D-H..H-X H48A ..H59	1.93 Ang.
	1+x,y,z =	1_655 Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O1 --H1	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O4 --H4	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O8 --H8	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O9 --H9	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O11 --H11	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O16 --H16	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O18 --H18	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O19 --H19	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O21 --H21	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O23 --H23	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O29 --H29	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O33 --H33	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O34 --H34	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O36 --H36	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O44 --H44	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O46 --H46	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O48 --H48	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O54 --H54	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O56 --H56	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O58 --H58	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O61 --H61	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O64 --H64	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O68 --H68	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O71 --H71	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O72 --H72	Please Check

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### ● Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

STRVA01\_ALERT\_4\_C Flack test results are ambiguous.

From the CIF: \_refine\_ls\_abs\_structure\_Flack 0.490

From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 0.160

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.29 Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C87 --C93	6.5 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O41 --C49	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O71 --C85	0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C85 --C92	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C91 --C92	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C97 --C98	0.18 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C89	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C90	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C93	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C85	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C87	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C88	Check

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C91	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	071	0.110 Check
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C87 - C93	1.70 Ang.
PLAT411_ALERT_2_C	Short	Inter H...H Contact	H10J ..H80A	2.10 Ang.
		x,y,z =	1_555	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#		1 Note
	C42 H70 O35			



### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
 usually due to the moiety formula being in the wrong format.  
 Atom count from \_chemical\_formula\_sum: C104 H172 O72  
 Atom count from \_chemical\_formula\_moiety: C52 H86 O36

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
 not performed for this radiation type.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		44	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero		0.490	Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		2.00	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		?	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure .....		!	Info
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C42 H70 O35			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C10 H16 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	C10 H16 O			
PLAT791_ALERT_4_G	Model has Chirality at C2	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C3	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C4	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C5	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C6	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C8	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C9	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C10	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C11	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C12	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C14	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C15	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C16	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C17	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C18	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C20	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C21	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C22	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C23	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C24	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C26	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C27	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C28	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C29	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C30	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C32	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C33	(Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C34	(Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C35	(Sohnke SpGr)	R	Verify

PLAT791_ALERT_4_G Model has Chirality at C36	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C38	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C39	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C40	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C41	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C42	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C44	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C45	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C46	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C47	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C48	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C50	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C51	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C52	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C53	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C54	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C56	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C57	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C58	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C59	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C60	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C62	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C63	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C64	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C65	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C66	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C68	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C69	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C70	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C71	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C72	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C74	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C75	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C76	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C77	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C78	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C80	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C81	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C82	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C83	(Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C84	(Sohnke SpGr)	R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....		4 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 !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...		16 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....		3.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged		Please Check

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 43 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 4 ALERT type 3 Indicator that the structure quality may be low  
 86 ALERT type 4 Improvement, methodology, query or suggestion  
 1 ALERT type 5 Informative message, check

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# checkCIF publication errors

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## 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.

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## Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

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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

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## 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.

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**PLATON version of 22/03/2021; check.def file version of 19/03/2021**

