

# 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 = 0.0098 A	Wavelength=0.71073
Cell:	a=19.1225(4)	b=24.2639(6)      c=32.6433(8)
	alpha=90	beta=90      gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	15146.1(6)	15146.0(6)
Space group	C 2 2 21	C 2 2 21
Hall group	C 2c 2	C 2c 2
Moiety formula	2(C42 H70 O35), 2(C5.50 H8.50 O) [+ solvent]	2(C42 H70 O35), 2(C5.50 H8.50 O) [+ SOLVENT]
Sum formula	C95 H157 O72 [+ solvent]	C95 H157 O72
Mr	2451.21	2451.20
Dx,g cm-3	1.075	1.075
Z	4	4
Mu (mm-1)	0.093	0.093
F000	5212.0	5212.0
F000'	5215.80	
h,k,lmax	22,28,38	22,28,38
Nref	13382[ 7205]	13052
Tmin,Tmax	0.970,0.974	0.970,0.974
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.970 Tmax=0.974  
AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.98      Theta(max)= 25.019

R(reflections)= 0.0883( 9831)      wR2(reflections)= 0.2859( 13052)

S = 1.153      Npar= 739

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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 A

PLAT097\_ALERT\_2\_A Large Reported Max. (Positive) Residual Density 1.82 eA-3

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### Alert level B

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for O30 --C36 . 11.2 s.u.  
PLAT416\_ALERT\_2\_B Short Intra D-H..H-D H3 ..H9 . 1.50 Ang.  
x,y,z = 1\_555 Check  
PLAT416\_ALERT\_2\_B Short Intra D-H..H-D H13 ..H19 . 1.47 Ang.  
x,y,z = 1\_555 Check  
PLAT417\_ALERT\_2\_B Short Inter D-H..H-D H8 ..H9 . 2.06 Ang.  
1-x,y,1/2-z = 4\_655 Check  
PLAT417\_ALERT\_2\_B Short Inter D-H..H-D H15 ..H30 . 2.00 Ang.  
-1/2+x,1/2+y,z = 5\_455 Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O5 --H50 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O10 --H10 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O15 --H15 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O35 --H35 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O51 --H510 . 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.

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.56 Report  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C36 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including O51 0.109 Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0098 Ang.  
PLAT417\_ALERT\_2\_C Short Inter D-H..H-D H240 ..H28 . 2.12 Ang.  
1-x,y,1/2-z = 4\_655 Check

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### 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: C95 H157 O72

Atom count from \_chemical\_formula\_moiety:C84 H140 O70

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 11 Note  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 22 Report  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
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 3 Report  
PLAT173\_ALERT\_4\_G The CIF-Embedded .res File Contains DANG Records 1 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O51 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O52 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C51 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C52 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C53 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C54 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C55 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C56 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C57 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C58 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C59 Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of C60	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C61	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H55A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H55B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H56	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H61A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H61B	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H20A ..H57B .		2.03 Ang.	
	x,y,z =	1_555	Check	
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure .....		!	Info
PLAT791_ALERT_4_G	Model has Chirality at C1 (Sohnke SpGr)		S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)		R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)		R	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 C7 (Sohnke SpGr)		S	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)		R	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 C13 (Sohnke SpGr)		S	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)		R	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 C19 (Sohnke SpGr)		S	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)		R	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 C25 (Sohnke SpGr)		S	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)		R	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 C31 (Sohnke SpGr)		S	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)		R	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 C37 (Sohnke SpGr)		S	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)		R	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
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 with s.u.		0.20	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		18	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 !

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
17 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  
70 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## 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.

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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.
```

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RESPONSE: ...
;
_vrf_PLAT097_I
;
PROBLEM: Large Reported Max. (Positive) Residual Density      1.82 eA-3
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**

Datablock I - ellipsoid plot

