

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

Bond precision: C-C = 0.0213 A Wavelength=0.71073

Cell: a=39.5857 (7) b=39.5857 (7) c=39.5857 (7)
 alpha=90 beta=90 gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	62032 (3)	62031.9 (19)
Space group	F d -3 m	Fd-3m
Hall group	-F 4vw 2vw	?
Moiety formula	C84 H36 N6 O28 Th3 [+ solvent]	?
Sum formula	C84 H36 N6 O28 Th3 [+ solvent]	C0 H0 N0 O0 Th48
Mr	2273.31	11137.92
Dx, g cm-3	0.974	0.298
Z	16	1
Mu (mm-1)	2.915	2.863
F000	17216.0	4320.0
F000'	16880.56	
h, k, lmax	47, 47, 47	40, 47, 41
Nref	2600	2599
Tmin, Tmax	0.759, 0.795	
Tmin'	0.744	

Correction method= Not given

Data completeness= 1.000 Theta (max)= 25.000

R(reflections)= 0.0673 (1478)

wR2(reflections)=
0.2128 (2599)

S = 0.969

Npar= 116

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 A

PLAT058_ALERT_1_A	Maximum Transmission Factor Missing	?
PLAT059_ALERT_1_A	Minimum Transmission Factor Missing	?
PLAT213_ALERT_2_A	Atom C2 has ADP max/min Ratio	5.4 prolat
PLAT213_ALERT_2_A	Atom C3 has ADP max/min Ratio	5.2 prolat
PLAT234_ALERT_4_A	Large Hirshfeld Difference C3 --C4 .	0.32 Ang.

Alert level B

PLAT220_ALERT_2_B	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	10.0 Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for C10 --C11 .	9.8 s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference O1 --C1 .	0.28 Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference C4 --C5 .	0.30 Ang.
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C10 Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	C11 Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.02131 Ang.
PLAT990_ALERT_1_B	Deprecated .res/.hkl Input Style SQUEEZE Job ...	! Note

Alert level C

ABSTY02_ALERT_1_C An `_exptl_absorpt_correction_type` has been given without a literature citation. This should be contained in the `_exptl_absorpt_process_details` field.
Absorption correction given as Multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.140

PLAT125_ALERT_4_C	No ' <code>_symmetry_space_group_name_Hall</code> ' Given	Please Do !
PLAT213_ALERT_2_C	Atom C1 has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C	Atom C4 has ADP max/min Ratio	3.1 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N1 --C6 .	7.0 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O4 --C6 .	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N1 --C7 .	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C7 --C8 .	0.20 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C3 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Th1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C2 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C6 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Th1	0.171 Check
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C10 - C10_k .	1.56 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the `_chemical_formula_sum` and the formula from the `_atom_site*` data.
Atom count from `_chemical_formula_sum`: Th48
Atom count from the `_atom_site` data: C1344 H576 N96 O448. Th48

CELLZ01_ALERT_1_G Difference between formula and `atom_site` contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_sum C0 H0 N0 O0 Th48
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff	
C	1.00	1344.00	-1343.00	
H	1.00	576.00	-575.00	
N	1.00	96.00	-95.00	
O	1.00	448.00	-447.00	
Th	48.00	48.00	0.00	

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	11	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.140	Report
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	16.00	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	1.82	%
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	11	Units
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C10 -C10_k .	1.43	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C10 -C10_k	0.22	Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C9 Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		! Info
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9 --C9	1.80	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Th1 (IV) .	4.13	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	94	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/	2018	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	7	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	6	Units

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 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
10 ALERT type 4 Improvement, methodology, query or suggestion
5 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.

● **Alert level G**

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

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

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: ...
;
_vrf_PLAT058_I
;
PROBLEM: Maximum Transmission Factor Missing ..... ?
RESPONSE: ...
;
_vrf_PLAT059_I
;
PROBLEM: Minimum Transmission Factor Missing ..... ?
RESPONSE: ...
;
_vrf_PLAT213_I
;
PROBLEM: Atom C2          has ADP max/min Ratio ..... 5.4 prolat
RESPONSE: ...
;
_vrf_PLAT234_I
;
PROBLEM: Large Hirshfeld Difference C3      --C4      .      0.32 Ang.
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 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot

