

checkCIF/PLATON report

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. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0094 Å

Wavelength=0.71073

Cell: a=10.9458(4) b=11.9419(4) c=13.4085(5)
 alpha=64.178(1) beta=79.870(2) gamma=77.179(1)
Temperature: 150 K

	Calculated	Reported
Volume	1532.06(10)	1532.06(10)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C40 H40 Ba2 N6 O15, 2(C12 H8 N2), 2(H2 O)	C40 H40 Ba2 N6 O15, 2(C12 H8 N2), 2(H2 O)
Sum formula	C64 H60 Ba2 N10 O17	C64 H60 Ba2 N10 O17
Mr	1515.88	1515.90
Dx, g cm ⁻³	1.643	1.643
Z	1	1
Mu (mm ⁻¹)	1.359	1.359
F000	762.0	762.0
F000'	761.68	
h,k,lmax	14,15,17	14,15,17
Nref	14070[7035]	13072
Tmin,Tmax	0.770,0.873	0.763,0.876
Tmin'	0.752	

Correction method= MULTI-SCAN

Data completeness= 1.86/0.93

Theta(max)= 27.480

R(reflections)= 0.0296(12197)

wR2(reflections)= 0.0597(13072)

S = 1.041

Npar= Npar = 904

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

PLAT417_ALERT_2_A	Short Inter D-H..H-D	H14W	..	H15W	..	1.40	Ang.
PLAT924_ALERT_1_A	The Reported and Calculated Rho(min) Differ by					8.45	eA-3
PLAT927_ALERT_1_A	Reported and Calculated wR2 Differ by					-0.0579	Check
PLAT974_ALERT_2_A	Check Calcd Negative Residual Density on			Ba2		-8.86	eA-3
PLAT974_ALERT_2_A	Check Calcd Negative Residual Density on			Ba1		-8.69	eA-3

🟡 Alert level B

PLAT420_ALERT_2_B	D-H Without Acceptor	O1W	-	H2W	...	Please	Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O3W	-	H6W	...	Please	Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O4W	-	H7W	...	Please	Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O5W	-	H10W	...	Please	Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O8W	-	H16W	...	Please	Check
PLAT910_ALERT_3_B	Missing # of FCF Reflections Below Th(Min)				17	Why ?
PLAT926_ALERT_1_B	Reported and Calculated R1 Differ by				-0.0244	Check
PLAT928_ALERT_1_B	Reported and Calculated S value Differ by					-1.008	

🟢 Alert level C

PLAT036_ALERT_1_C	No s.u. Given for Flack Parameter					Please	Do !
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)					7.74	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density				2.06	Why ?
PLAT213_ALERT_2_C	Atom N1		has	ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C	Atom C61		has	ADP max/min Ratio	3.8	prolat
PLAT220_ALERT_2_C	Large Non-Solvent N		Ueq(max)/Ueq(min) Range			3.5	Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H		Uiso(max)/Uiso(min)		..	5.5	Ratio
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for		C60	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor				3.0	Note
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O1W			-H2W		84.22	Degree
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O3W			-H6W		88.32	Degree
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O7W			-H14W		80.69	Degree
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds				0.0094	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C9	-	C10	...	1.55	Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H5W	..	H17W	..	2.12	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H2W	..	O2W	..	2.61	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H3W	..	O1W	..	2.66	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H5W	..	N9	..	2.68	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H9W	..	N10	..	2.70	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H14W	..	O4W	..	2.63	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H16W	..	O2W	..	2.65	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=			0.600		17	Why ?
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF				2	Note
PLAT915_ALERT_3_C	Low Friedel Pair Coverage				86	%
PLAT975_ALERT_2_C	Check Calcd Residual Density	0.82A	From	O2		0.55	eA-3

🟠 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					33	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension				1	Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF					Please	Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical					?	Check
PLAT111_ALERT_2_G	ADDSYM Detects (Pseudo) Centre of Symmetry				81	%Fit
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range	C56	-	C61		0.16	Ang.
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					210	Do !
	O7 -BA2 -O6 -C9	-8.80	1.00	1.655	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					317	Do !
	BA2 -C16 -C12 -C11	-119.10	1.90	1.455	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					320	Do !
	BA2 -C16 -C12 -C13	57.00	2.00	1.455	1.555	1.555	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.				#	3	Note

C12 H8 N2	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	5 Note
H2 O	
PLAT860_ALERT_3_G Number of Least-Squares Restraints	36 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	12 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by .	0.31 Check

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

6 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
8 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

```
# 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_PLAT417_I
;
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PROBLEM: Short Inter D-H..H-D      H14W   ..  H15W   ..      1.40 Ang.
RESPONSE: ...
;
_vrf_PLAT924_I
;
PROBLEM: The Reported and Calculated Rho(min) Differ by .      8.45 eA-3
RESPONSE: ...
;
_vrf_PLAT927_I
;
PROBLEM: Reported and Calculated  wR2 Differ by .....      -0.0579 Check
RESPONSE: ...
;
_vrf_PLAT974_I
;
PROBLEM: Check Calcd Negative Residual Density on      Ba2      -8.86 eA-3
RESPONSE: ...
;
# end Validation Reply Form

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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 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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