

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Br2-OTO, o-Br2-DBTO, o-Br2-DBTO2

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: o-Br2-DBTO

Bond precision:	C-C = 0.0025 A	Wavelength=0.71073	
Cell:	a=7.6547 (4)	b=8.0798 (4)	c=18.3175 (11)
	alpha=90	beta=95.204 (3)	gamma=90
Temperature:	193 K		

	Calculated	Reported
Volume	1128.24 (11)	1128.24 (11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C12 H6 Br2 O S	C12 H6 Br2 O S
Sum formula	C12 H6 Br2 O S	C12 H6 Br2 O S
Mr	358.03	358.03
Dx, g cm ⁻³	2.108	2.108
Z	4	4
Mu (mm ⁻¹)	7.341	7.341
F000	688.0	688.0
F000'	686.58	
h, k, l _{max}	10, 11, 25	10, 11, 25
Nref	3181	3176
Tmin, Tmax	0.254, 0.480	0.445, 0.746
Tmin'	0.221	

Correction method= # Reported T Limits: Tmin=0.445 Tmax=0.746
AbsCorr = MULTI-SCAN


Data completeness= 0.998 Theta (max)= 29.627

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R(reflections)= 0.0222( 2729)      wR2(reflections)=
S = 1.026                        0.0512( 3176)
Npar= 145
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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.

 Alert level G		
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1 Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 1 1, 0 0 2,	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 3 1 3,	1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.8 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value Predicted wR2: Based on SigI**2 2.63 or SHELX Weight 4.99	1.944 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **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
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

Datablock: Br2-OTO

Bond precision: C-C = 0.0056 A Wavelength=0.71073

Cell: a=14.908(6) b=14.778(9) c=11.443(4)
alpha=90 beta=109.731(10) gamma=90

Temperature: 193 K

	Calculated	Reported
Volume	2373.0(19)	2373.0(19)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H6 Br2 O2 S	C12 H6 Br2 O2 S
Sum formula	C12 H6 Br2 O2 S	C12 H6 Br2 O2 S
Mr	374.03	374.03
Dx, g cm ⁻³	2.094	2.094
Z	8	8
Mu (mm ⁻¹)	6.992	6.991
F000	1440.0	1440.0
F000'	1437.22	
h,k,lmax	18,18,14	18,18,14
Nref	4613	4603
Tmin,Tmax	0.516,0.657	0.568,0.745
Tmin'	0.324	

Correction method= # Reported T Limits: Tmin=0.568 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.938

R(reflections)= 0.0325(3749) wR2(reflections)=
0.0817(4603)
S = 1.033 Npar= 307

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 G

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters	1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	4 Note
1 0 0, 1 1 0, -1 1 1, 0 1 1,	
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	8 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	2.116 Note
Predicted wR2: Based on SigI**2 3.86 or SHELX Weight 7.90	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	7 Info

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- 0 **ALERT level B** = A potentially serious problem, consider carefully
- 0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 5 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: o-Br2-DBTO2

Bond precision: C-C = 0.0033 Å

Wavelength=0.71073

Cell: a=7.7340 (9) b=12.7252 (16) c=13.8282 (18)
alpha=116.240 (4) beta=99.561 (5) gamma=97.142 (5)
Temperature: 193 K

	Calculated	Reported
Volume	1173.3 (3)	1173.3 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H6 Br2 O2 S	C12 H6 Br2 O2 S
Sum formula	C12 H6 Br2 O2 S	C12 H6 Br2 O2 S
Mr	374.03	374.03
Dx, g cm ⁻³	2.117	2.117
Z	4	4
Mu (mm ⁻¹)	7.070	7.071
F000	720.0	720.0
F000'	718.61	
h, k, lmax	11, 19, 21	11, 19, 21
Nref	9017	8940
Tmin, Tmax	0.512, 0.868	0.498, 0.747
Tmin'	0.277	

Correction method= # Reported T Limits: Tmin=0.498 Tmax=0.747

AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 33.224

R(reflections)= 0.0308 (6519)

wR2(reflections)=
0.0710 (8940)

S = 1.002

Npar= 307

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 C

PLAT431_ALERT_2_C Short Inter HL..A Contact Br4 ..02 . 3.13 Ang.
 x,y,-1+z = 1_554 Check



Alert level G

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
 0 1 0, 0 -1 1, 0 0 1,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 73 Note
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.646 Note
 Predicted wR2: Based on SigI**2 4.32 or SHELX Weight 7.09
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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- 2 ALERT type 4 Improvement, methodology, query or suggestion
- 1 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: ...
;
# 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 13/05/2024; check.def file version of 04/05/2024

Datablock o-Br2-DBTO - ellipsoid plot

